



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 04:57 PM UTC

PDB ID : 3JD8 / pdb_00003jd8
EMDB ID : EMD-6640
Title : cryo-EM structure of the full-length human NPC1 at 4.4 angstrom
Authors : Gong, X.; Qian, H.W.; Zhou, X.H.; Wu, J.P.; Zhou, Q.; Yan, N.
Deposited on : 2016-05-01
Resolution : 4.43 Å(reported)
Based on initial models : 3GKI, 5F1B

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

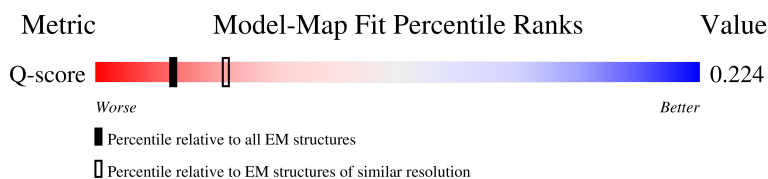
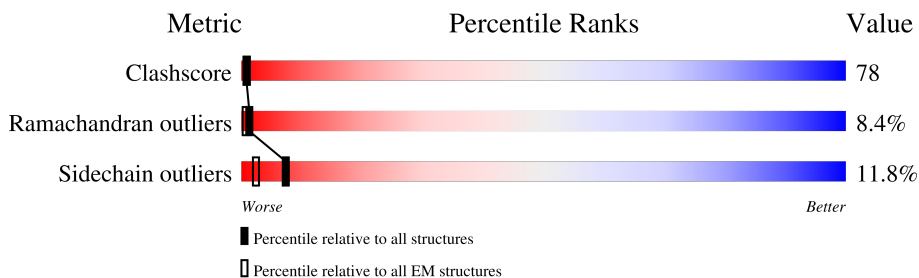
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.43 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	3083 (3.93 - 4.93)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1278	18% 47% 30% 10% 11%
2	B	2	100% 100%
2	C	2	50% 50% 50%
2	E	2	50% 50%

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Mol	Chain	Length	Quality of chain
3	D	3	 100%
4	F	4	 100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	D	1	-	-	X	-
3	NAG	D	2	-	-	X	-
4	NAG	F	1	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 8050 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Niemann-Pick C1 protein.

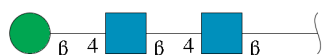
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1133	Total	C	N	O	S	1	0
			7695	4862	1315	1476	42		

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



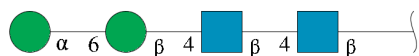
Mol	Chain	Residues	Atoms				AltConf	Trace
2	B	2	Total	C	N	O	0	0
			28	16	2	10		
2	C	2	Total	C	N	O	0	0
			28	16	2	10		
2	E	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



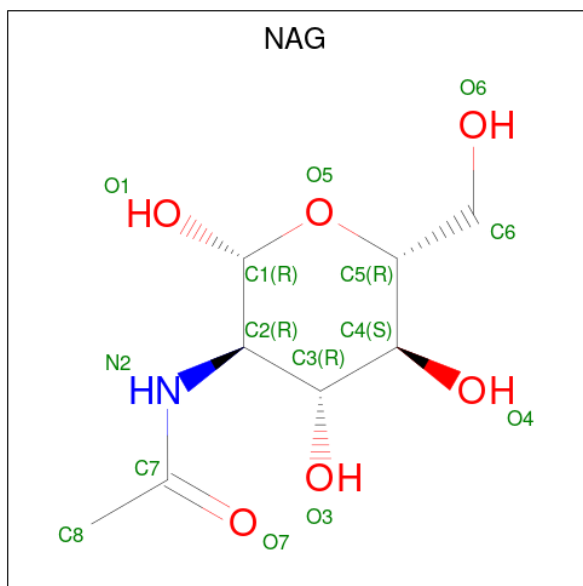
Mol	Chain	Residues	Atoms				AltConf	Trace
3	D	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
4	F	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



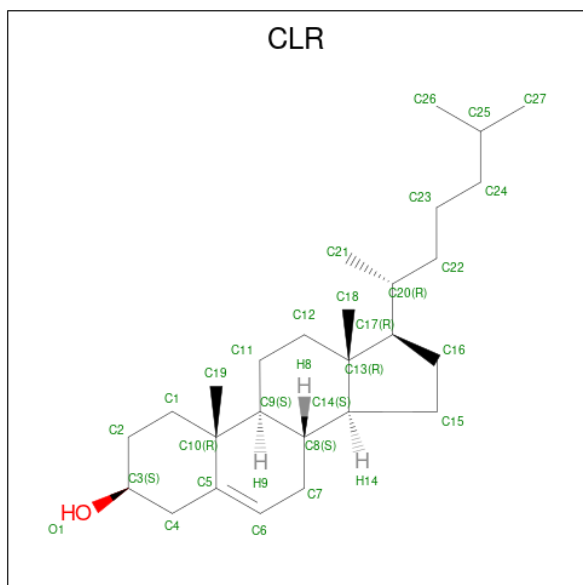
Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	

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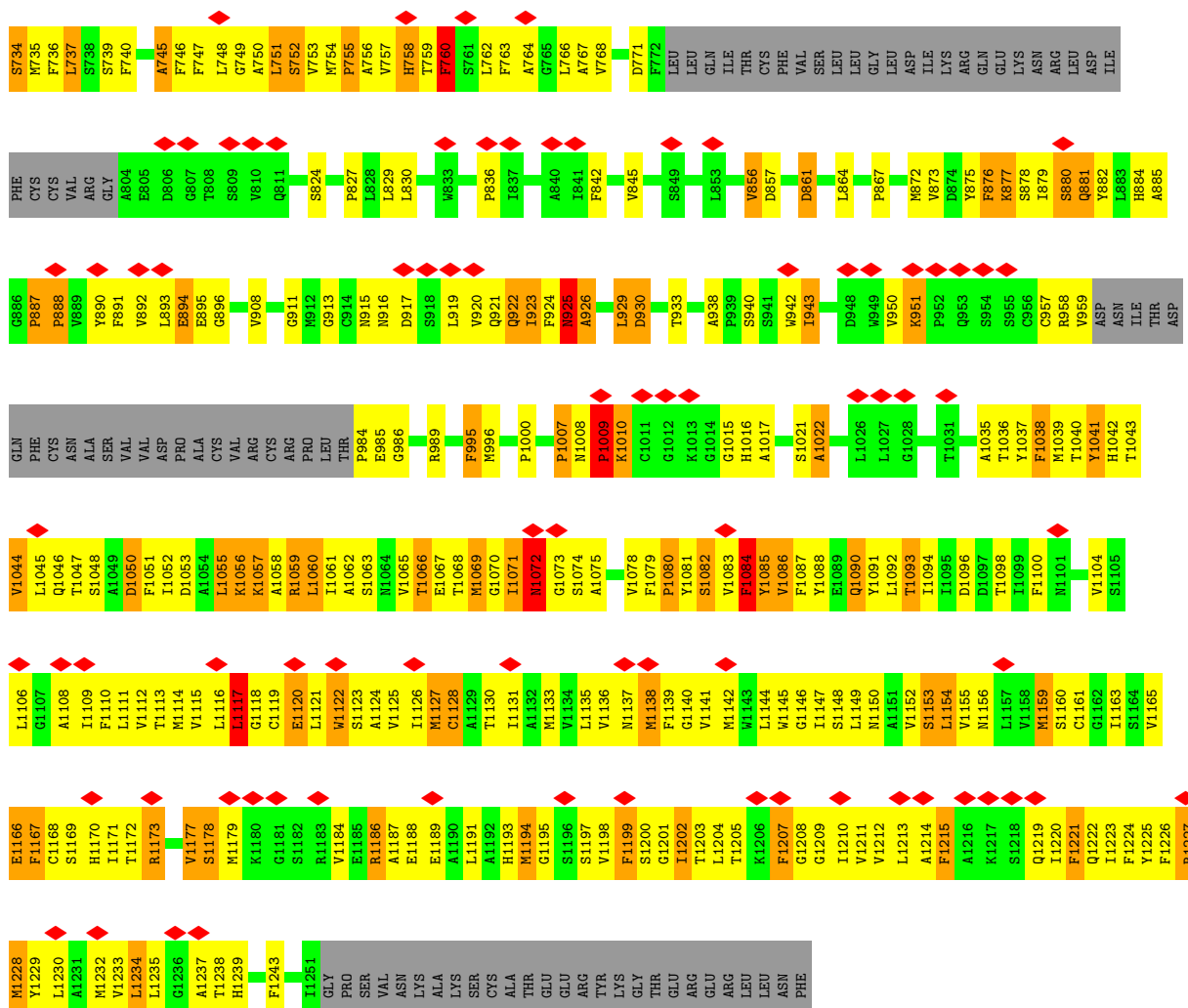
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Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 6 is CHOLESTEROL (CCD ID: CLR) (formula: $C_{27}H_{46}O$).



Mol	Chain	Residues	Atoms			AltConf
6	A	1	Total	C	O	0
			28	27	1	



- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 4: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	102731	Depositor
Resolution determination method	Not provided	
CTF correction method	Each micrograph	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	38270	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.087	Depositor
Minimum map value	-0.037	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.025	Depositor
Map size ($\text{\AA}$)	261.308, 261.308, 261.308	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.30654, 1.30654, 1.30654	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, CLR, MAN, NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.69	23/7843 (0.3%)	0.98	58/10748 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	940	SER	C-N	23.20	1.66	1.33
1	A	469	LEU	C-N	-9.37	1.22	1.33
1	A	1060	LEU	C-N	8.56	1.44	1.33
1	A	881	GLN	C-N	-8.32	1.22	1.33
1	A	884	HIS	C-N	-7.99	1.23	1.33
1	A	429	VAL	C-N	-7.64	1.23	1.33
1	A	602	SER	N-CA	6.50	1.54	1.45
1	A	252	GLN	C-N	6.40	1.41	1.33
1	A	253	PRO	C-N	6.33	1.40	1.33
1	A	254	PRO	C-N	6.27	1.40	1.33
1	A	671	SER	CA-C	5.97	1.60	1.52
1	A	602	SER	CA-C	5.56	1.59	1.52
1	A	166	PRO	N-CD	5.34	1.55	1.47
1	A	424	PRO	N-CD	5.12	1.55	1.47
1	A	249	PRO	N-CD	5.11	1.55	1.47
1	A	401	PRO	N-CD	5.08	1.54	1.47
1	A	254	PRO	N-CD	5.06	1.54	1.47
1	A	255	PRO	N-CD	5.05	1.54	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	253	PRO	N-CD	5.04	1.54	1.47
1	A	384	PRO	N-CD	5.04	1.54	1.47
1	A	251	PRO	N-CD	5.03	1.54	1.47
1	A	422	PRO	N-CD	5.01	1.54	1.47
1	A	691	PRO	N-CD	5.00	1.54	1.47

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	881	GLN	N-CA-C	10.40	123.53	108.86
1	A	995	PHE	N-CA-C	10.34	121.88	108.34
1	A	429	VAL	O-C-N	-8.87	110.99	121.10
1	A	602	SER	CB-CA-C	-8.62	91.11	110.07
1	A	996	MET	CA-C-N	-8.60	105.11	121.54
1	A	996	MET	C-N-CA	-8.60	105.11	121.54
1	A	755	PRO	CA-N-CD	-8.58	99.99	112.00
1	A	671	SER	N-CA-C	8.46	121.35	107.73
1	A	248	GLY	C-N-CD	8.45	139.19	120.60
1	A	603	PHE	N-CA-C	8.42	123.58	109.76
1	A	423	TYR	C-N-CD	8.42	139.13	120.60
1	A	887	PRO	N-CA-CB	8.36	111.18	103.08
1	A	940	SER	CA-C-N	-7.53	107.16	121.54
1	A	940	SER	C-N-CA	-7.53	107.16	121.54
1	A	363	ALA	N-CA-C	7.03	118.83	111.03
1	A	254	PRO	CA-C-N	-6.98	113.19	120.38
1	A	254	PRO	C-N-CA	-6.98	113.19	120.38
1	A	1009	PRO	N-CA-CB	6.94	110.53	103.25
1	A	253	PRO	CA-C-N	-6.89	113.28	120.38
1	A	253	PRO	C-N-CA	-6.89	113.28	120.38
1	A	252	GLN	CA-C-N	-6.86	113.31	120.38
1	A	252	GLN	C-N-CA	-6.86	113.31	120.38
1	A	377	PRO	N-CA-CB	6.86	110.45	103.25
1	A	752	SER	N-CA-C	6.86	119.76	111.40
1	A	1007	PRO	N-CA-CB	6.81	110.40	103.25
1	A	733	PRO	N-CA-CB	6.79	110.39	103.25
1	A	888	PRO	N-CA-CB	6.79	110.37	103.25
1	A	350	PRO	N-CA-CB	6.78	110.37	103.25
1	A	836	PRO	N-CA-CB	6.77	111.02	103.44
1	A	867	PRO	N-CA-CB	6.65	110.40	103.15
1	A	1000	PRO	N-CA-CB	6.62	110.37	103.15
1	A	827	PRO	N-CA-CB	6.49	110.40	103.52
1	A	602	SER	N-CA-C	6.04	118.36	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	469	LEU	O-C-N	5.84	130.41	122.82
1	A	752	SER	CB-CA-C	-5.67	101.26	110.79
1	A	165	ALA	CA-C-N	-5.47	113.00	119.84
1	A	165	ALA	C-N-CA	-5.47	113.00	119.84
1	A	363	ALA	CB-CA-C	-5.38	102.62	110.95
1	A	256	PRO	CA-N-CD	-5.24	104.66	112.00
1	A	383	ALA	CA-C-N	-5.23	113.30	119.84
1	A	383	ALA	C-N-CA	-5.23	113.30	119.84
1	A	421	GLN	CA-C-N	-5.21	113.33	119.84
1	A	421	GLN	C-N-CA	-5.21	113.33	119.84
1	A	400	GLY	CA-C-N	-5.20	113.35	119.84
1	A	400	GLY	C-N-CA	-5.20	113.35	119.84
1	A	690	ILE	CA-C-N	-5.17	113.38	119.84
1	A	690	ILE	C-N-CA	-5.17	113.38	119.84
1	A	938	ALA	O-C-N	5.14	125.05	120.48
1	A	469	LEU	CA-C-N	-5.13	115.91	123.30
1	A	469	LEU	C-N-CA	-5.13	115.91	123.30
1	A	259	PRO	CA-N-CD	-5.10	104.86	112.00
1	A	256	PRO	CA-C-N	-5.09	113.48	119.84
1	A	256	PRO	C-N-CA	-5.09	113.48	119.84
1	A	925	ASN	CA-C-N	5.08	131.23	121.54
1	A	925	ASN	C-N-CA	5.08	131.23	121.54
1	A	470	ALA	CA-C-N	5.04	124.83	119.28
1	A	470	ALA	C-N-CA	5.04	124.83	119.28
1	A	257	PRO	CA-N-CD	-5.01	104.99	112.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	602	SER	Peptide
1	A	603	PHE	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7695	0	6477	1135	0
2	B	28	0	25	0	0
2	C	28	0	25	3	0
2	E	28	0	25	4	0
3	D	39	0	34	19	0
4	F	50	0	43	10	0
5	A	154	0	142	17	0
6	A	28	0	46	1	0
All	All	8050	0	6817	1158	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 78.

All (1158) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:598:ASN:HD21	2:E:1:NAG:C1	0.99	1.62
1:A:724:LEU:HD22	1:A:1170:HIS:CE1	1.29	1.62
1:A:1138:MET:HE2	1:A:1232:MET:CB	1.20	1.56
1:A:656:LEU:CD1	1:A:685:ILE:HG13	1.17	1.56
1:A:524:ASN:ND2	2:C:1:NAG:C1	1.68	1.54
1:A:656:LEU:HD11	1:A:685:ILE:CG1	1.31	1.52
1:A:693:LEU:HD11	1:A:763:PHE:CE2	1.41	1.52
1:A:158:ASN:ND2	5:A:1303:NAG:C1	1.69	1.50
1:A:70:ASN:HD21	5:A:1317:NAG:C1	1.26	1.49
1:A:185:ASN:HD21	5:A:1319:NAG:C1	1.24	1.48
1:A:403:PHE:CE2	1:A:566:PRO:HB3	1.46	1.46
1:A:684:LEU:CD2	1:A:728:LEU:HD13	1.45	1.44
1:A:659:ALA:HA	1:A:662:LEU:CD2	1.46	1.44
1:A:693:LEU:CD1	1:A:763:PHE:HE2	1.30	1.43
1:A:631:MET:CE	1:A:1204:LEU:O	1.64	1.42
1:A:693:LEU:HD11	1:A:763:PHE:CD2	1.52	1.42
1:A:1133:MET:HG2	1:A:1239:HIS:NE2	1.12	1.42
1:A:185:ASN:ND2	5:A:1319:NAG:C1	1.80	1.42
1:A:1133:MET:HG2	1:A:1239:HIS:CD2	1.52	1.42
1:A:135:ASN:ND2	5:A:1322:NAG:C1	1.81	1.41
1:A:656:LEU:CD1	1:A:685:ILE:CG1	1.85	1.40
1:A:1178:SER:CB	1:A:1186:ARG:HH11	1.35	1.40
1:A:684:LEU:HD21	1:A:728:LEU:CD1	1.51	1.38
1:A:598:ASN:ND2	2:E:1:NAG:C1	1.85	1.37
1:A:688:GLU:CG	1:A:724:LEU:HD23	1.52	1.35
1:A:688:GLU:O	1:A:691:PRO:HD2	1.20	1.35

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:684:LEU:HD21	1:A:728:LEU:CD2	1.55	1.34
1:A:693:LEU:CD1	1:A:763:PHE:CE2	2.03	1.33
1:A:723:GLN:OE1	1:A:1169:SER:HB2	1.20	1.33
1:A:1133:MET:HE2	1:A:1239:HIS:ND1	1.05	1.33
1:A:523:LEU:HD11	1:A:1016:HIS:CB	1.58	1.32
1:A:724:LEU:CD2	1:A:1170:HIS:CE1	2.13	1.31
1:A:401:PRO:HD3	1:A:571:TYR:CE1	1.65	1.31
1:A:1142:MET:HA	1:A:1147:ILE:CB	1.57	1.31
1:A:856:VAL:CB	1:A:1091:TYR:HE2	1.41	1.30
1:A:686:VAL:HG12	1:A:690:ILE:CD1	1.62	1.30
1:A:1133:MET:CE	1:A:1239:HIS:ND1	1.95	1.29
1:A:557:ASN:ND2	3:D:1:NAG:C1	1.96	1.29
1:A:1084:PHE:CE1	1:A:1085:TYR:CD1	2.20	1.29
1:A:1138:MET:CE	1:A:1232:MET:HB2	1.63	1.28
1:A:401:PRO:HG3	1:A:571:TYR:CD1	1.68	1.28
1:A:923:ILE:O	1:A:1042:HIS:HB2	1.33	1.28
1:A:1142:MET:HE3	1:A:1148:SER:O	1.11	1.28
1:A:452:ASN:HD21	5:A:1323:NAG:C1	1.45	1.28
1:A:926:ALA:O	1:A:1040:THR:HG22	1.34	1.28
1:A:686:VAL:CG1	1:A:690:ILE:HD11	1.61	1.27
1:A:70:ASN:ND2	5:A:1317:NAG:C1	1.95	1.26
1:A:1070:GLY:O	1:A:1071:ILE:CG1	1.83	1.26
1:A:459:ASN:ND2	5:A:1324:NAG:C1	1.97	1.26
1:A:923:ILE:O	1:A:1042:HIS:CB	1.83	1.26
1:A:648:LEU:HB3	1:A:763:PHE:CE1	1.70	1.26
1:A:751:LEU:O	1:A:755:PRO:HG3	1.29	1.25
1:A:659:ALA:CA	1:A:662:LEU:HD23	1.66	1.24
1:A:162:ASP:OD2	1:A:244:SER:CB	1.86	1.24
1:A:406:GLU:OE1	1:A:583:TRP:HZ3	1.17	1.23
1:A:688:GLU:HG2	1:A:1170:HIS:NE2	1.54	1.23
1:A:724:LEU:HD22	1:A:1170:HIS:NE2	1.54	1.23
1:A:684:LEU:CD2	1:A:728:LEU:CD1	2.09	1.22
1:A:1055:LEU:HD23	1:A:1085:TYR:CZ	1.73	1.22
1:A:1138:MET:CE	1:A:1232:MET:CB	2.15	1.22
1:A:452:ASN:ND2	5:A:1323:NAG:C1	2.02	1.21
1:A:478:ASN:HD21	4:F:1:NAG:C1	1.52	1.21
1:A:915:ASN:CB	1:A:920:VAL:HA	1.69	1.21
1:A:688:GLU:O	1:A:691:PRO:CD	1.86	1.21
1:A:676:SER:HB3	1:A:1225:TYR:OH	1.41	1.20
1:A:856:VAL:O	1:A:1048:SER:CB	1.89	1.20
1:A:162:ASP:OD2	1:A:244:SER:HB3	1.04	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:LYS:HB3	1:A:251:PRO:CD	1.70	1.20
1:A:882:TYR:CB	1:A:1082:SER:HB3	1.70	1.19
1:A:684:LEU:HD21	1:A:728:LEU:CG	1.70	1.19
1:A:1133:MET:HE2	1:A:1239:HIS:CG	1.76	1.19
1:A:924:PHE:H	1:A:925:ASN:CB	1.56	1.18
1:A:1127:MET:CE	1:A:1168:CYS:HB3	1.74	1.18
1:A:1133:MET:CG	1:A:1239:HIS:CD2	2.26	1.17
1:A:755:PRO:HD2	1:A:756:ALA:H	1.06	1.16
1:A:1142:MET:CA	1:A:1147:ILE:CB	2.22	1.16
1:A:732:ALA:CB	1:A:749:GLY:HA3	1.75	1.16
1:A:767:ALA:O	1:A:771:ASP:CB	1.94	1.16
1:A:1108:ALA:O	1:A:1112:VAL:HG23	1.43	1.16
1:A:730:GLU:CG	1:A:1108:ALA:HB1	1.76	1.16
1:A:1133:MET:CG	1:A:1239:HIS:NE2	2.08	1.16
1:A:1133:MET:HG2	1:A:1239:HIS:CE1	1.81	1.15
1:A:656:LEU:HD11	1:A:685:ILE:CB	1.77	1.15
1:A:1178:SER:CB	1:A:1186:ARG:HD2	1.76	1.15
1:A:959:VAL:CB	1:A:984:PRO:N	2.10	1.15
1:A:1138:MET:CE	1:A:1232:MET:HA	1.76	1.14
1:A:1142:MET:CE	1:A:1148:SER:O	1.93	1.14
1:A:1071:ILE:O	1:A:1072:ASN:O	1.65	1.14
1:A:1084:PHE:CE1	1:A:1085:TYR:HD1	1.59	1.14
1:A:507:ALA:HB1	1:A:529:LEU:HG	1.28	1.14
1:A:724:LEU:CD1	1:A:1166:GLU:HG2	1.77	1.14
1:A:1009:PRO:HA	1:A:1016:HIS:O	1.44	1.13
1:A:1178:SER:CB	1:A:1186:ARG:CD	2.25	1.13
1:A:1127:MET:HA	1:A:1127:MET:HE3	1.17	1.13
1:A:1138:MET:HE1	1:A:1232:MET:HA	1.23	1.13
1:A:635:ILE:HG23	1:A:690:ILE:HD13	1.14	1.13
1:A:631:MET:SD	1:A:1208:GLY:CA	2.36	1.13
1:A:1070:GLY:O	1:A:1071:ILE:HG13	0.95	1.12
1:A:1138:MET:HE2	1:A:1232:MET:CA	1.76	1.12
1:A:135:ASN:HD21	5:A:1322:NAG:C1	1.50	1.12
1:A:1140:GLY:O	1:A:1144:LEU:CB	1.96	1.12
1:A:720:LEU:HD22	1:A:1170:HIS:HA	1.29	1.12
1:A:1046:GLN:CB	1:A:1050:ASP:OD2	1.98	1.12
1:A:752:SER:O	1:A:755:PRO:HD2	1.46	1.11
1:A:856:VAL:O	1:A:1048:SER:HB3	1.44	1.11
1:A:684:LEU:CD2	1:A:728:LEU:HD22	1.79	1.11
1:A:879:ILE:CA	1:A:1043:THR:HG21	1.79	1.11
1:A:688:GLU:HG3	1:A:724:LEU:HD23	1.29	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:GLU:OE1	1:A:583:TRP:CZ3	2.03	1.10
1:A:724:LEU:HD11	1:A:1166:GLU:CG	1.81	1.10
1:A:659:ALA:C	1:A:662:LEU:HD23	1.76	1.10
1:A:752:SER:O	1:A:755:PRO:CD	1.99	1.10
1:A:1178:SER:CB	1:A:1186:ARG:NH1	2.14	1.10
1:A:656:LEU:CB	1:A:682:LEU:HD11	1.79	1.10
1:A:1098:THR:HG22	1:A:1154:LEU:HD21	1.22	1.09
1:A:688:GLU:C	1:A:691:PRO:CD	2.23	1.09
1:A:856:VAL:CB	1:A:1091:TYR:CE2	2.34	1.09
1:A:915:ASN:CA	1:A:920:VAL:HA	1.81	1.09
1:A:688:GLU:HG2	1:A:724:LEU:HD23	1.32	1.09
1:A:1138:MET:CE	1:A:1232:MET:CA	2.31	1.09
1:A:1062:ALA:HB1	1:A:1078:VAL:HB	1.18	1.09
1:A:631:MET:HE1	1:A:1204:LEU:C	1.77	1.08
1:A:403:PHE:CD2	1:A:566:PRO:HB3	1.87	1.08
3:D:2:NAG:H62	3:D:3:BMA:C2	1.82	1.08
1:A:365:SER:HA	1:A:662:LEU:HB3	1.30	1.08
1:A:684:LEU:HD23	1:A:728:LEU:HD13	1.14	1.08
1:A:687:ILE:O	1:A:691:PRO:HD3	1.53	1.08
1:A:730:GLU:HG3	1:A:1108:ALA:CB	1.82	1.08
1:A:929:LEU:CB	1:A:1038:PHE:CD2	2.37	1.08
1:A:196:LYS:HG3	1:A:204:THR:OG1	1.54	1.07
1:A:680:LEU:HB3	1:A:1229:TYR:OH	1.50	1.07
1:A:879:ILE:C	1:A:1043:THR:CG2	2.28	1.07
1:A:228:ASP:CB	1:A:246:VAL:HG13	1.84	1.07
1:A:607:ARG:HG2	1:A:611:ASP:CG	1.79	1.07
1:A:656:LEU:HD13	1:A:685:ILE:HG13	1.26	1.07
1:A:403:PHE:HE2	1:A:566:PRO:CB	1.67	1.06
1:A:1071:ILE:CG2	1:A:1072:ASN:H	1.62	1.06
1:A:684:LEU:CD2	1:A:728:LEU:CD2	2.33	1.06
1:A:685:ILE:O	1:A:689:VAL:HG23	1.56	1.06
1:A:923:ILE:C	1:A:1042:HIS:HB3	1.80	1.05
1:A:1142:MET:O	1:A:1147:ILE:CB	2.02	1.05
1:A:1062:ALA:HB1	1:A:1078:VAL:CB	1.86	1.05
1:A:478:ASN:ND2	4:F:1:NAG:C1	2.17	1.05
1:A:688:GLU:C	1:A:691:PRO:HD3	1.82	1.05
1:A:879:ILE:C	1:A:1043:THR:HG22	1.81	1.05
1:A:403:PHE:CE2	1:A:566:PRO:CB	2.40	1.04
1:A:631:MET:HE1	1:A:1204:LEU:O	0.88	1.04
1:A:1133:MET:CE	1:A:1239:HIS:CG	2.39	1.04
1:A:635:ILE:HG23	1:A:690:ILE:CD1	1.86	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:635:ILE:CG2	1:A:690:ILE:CD1	2.35	1.04
1:A:732:ALA:CB	1:A:749:GLY:CA	2.35	1.03
1:A:656:LEU:HD13	1:A:685:ILE:CG1	1.74	1.03
1:A:879:ILE:N	1:A:1043:THR:HG21	1.71	1.03
1:A:717:GLY:O	1:A:721:ASP:HB2	1.58	1.03
1:A:1194:MET:HE3	1:A:1194:MET:HA	1.39	1.03
1:A:1065:VAL:O	1:A:1068:THR:HG22	1.56	1.03
1:A:1156:ASN:HB3	1:A:1228:MET:CE	1.87	1.03
1:A:631:MET:SD	1:A:1208:GLY:N	2.32	1.03
1:A:659:ALA:HA	1:A:662:LEU:HD23	1.13	1.03
1:A:688:GLU:HG2	1:A:724:LEU:CD2	1.87	1.02
1:A:751:LEU:O	1:A:755:PRO:CG	2.05	1.02
1:A:686:VAL:CG1	1:A:690:ILE:CD1	2.27	1.02
1:A:915:ASN:HA	1:A:920:VAL:HA	1.38	1.02
1:A:924:PHE:N	1:A:925:ASN:CB	2.22	1.02
1:A:523:LEU:CD1	1:A:1016:HIS:CB	2.36	1.02
1:A:648:LEU:HD12	1:A:763:PHE:CD1	1.95	1.02
1:A:656:LEU:HB2	1:A:682:LEU:CD1	1.88	1.02
1:A:688:GLU:CG	1:A:724:LEU:CD2	2.38	1.02
1:A:1084:PHE:CE1	1:A:1085:TYR:CE1	2.47	1.02
1:A:879:ILE:CA	1:A:1043:THR:CG2	2.38	1.01
1:A:1046:GLN:HB3	1:A:1050:ASP:OD2	1.59	1.01
1:A:337:ARG:HA	1:A:718:GLU:HG3	1.41	1.01
1:A:1071:ILE:HG22	1:A:1072:ASN:N	1.61	1.01
1:A:1138:MET:HE3	1:A:1138:MET:HA	1.40	1.01
1:A:752:SER:C	1:A:755:PRO:CD	2.33	1.01
3:D:2:NAG:C6	3:D:3:BMA:H2	1.90	1.01
1:A:401:PRO:CD	1:A:571:TYR:CE1	2.44	1.00
1:A:635:ILE:HG21	1:A:690:ILE:HD11	1.40	1.00
1:A:693:LEU:HD12	1:A:763:PHE:HE2	1.18	1.00
1:A:929:LEU:CB	1:A:1038:PHE:CE2	2.45	1.00
1:A:1142:MET:C	1:A:1147:ILE:CB	2.35	1.00
1:A:723:GLN:OE1	1:A:1169:SER:CB	2.08	1.00
1:A:401:PRO:HB2	1:A:569:ASN:ND2	1.75	0.99
1:A:1209:GLY:HA3	1:A:1230:LEU:HD13	1.43	0.99
1:A:922:GLN:O	1:A:1042:HIS:ND1	1.93	0.99
3:D:2:NAG:H62	3:D:3:BMA:H2	0.99	0.99
1:A:402:PHE:O	1:A:403:PHE:HB3	1.63	0.99
1:A:250:LYS:HB3	1:A:251:PRO:HD3	1.38	0.99
1:A:659:ALA:CA	1:A:662:LEU:CD2	2.28	0.99
1:A:686:VAL:HG12	1:A:690:ILE:HD12	1.42	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:732:ALA:HB3	1:A:749:GLY:HA3	1.40	0.98
1:A:1062:ALA:HA	1:A:1078:VAL:HG21	1.44	0.98
1:A:1127:MET:HE1	1:A:1168:CYS:HB3	1.38	0.98
1:A:656:LEU:HB2	1:A:682:LEU:HD11	0.98	0.98
1:A:684:LEU:CD1	1:A:1166:GLU:HG3	1.93	0.98
1:A:724:LEU:HD22	1:A:1170:HIS:HE1	1.21	0.98
1:A:1045:LEU:HA	1:A:1051:PHE:CZ	1.99	0.98
1:A:459:ASN:HD21	5:A:1324:NAG:C1	1.66	0.98
1:A:1127:MET:CE	1:A:1127:MET:HA	1.94	0.98
1:A:677:TYR:O	1:A:681:PRO:CB	2.12	0.97
1:A:1071:ILE:HG22	1:A:1072:ASN:H	0.83	0.97
1:A:1156:ASN:ND2	1:A:1228:MET:HE3	1.79	0.97
1:A:680:LEU:CB	1:A:1229:TYR:OH	2.13	0.97
1:A:676:SER:OG	1:A:1226:PHE:CE2	2.15	0.97
1:A:724:LEU:CD2	1:A:1170:HIS:NE2	2.22	0.97
1:A:1138:MET:HE2	1:A:1232:MET:HB3	1.46	0.97
1:A:557:ASN:HD21	3:D:1:NAG:C1	1.72	0.97
1:A:1045:LEU:HA	1:A:1051:PHE:HZ	1.27	0.96
1:A:607:ARG:O	1:A:611:ASP:N	1.98	0.96
1:A:732:ALA:HB1	1:A:749:GLY:HA3	1.45	0.96
1:A:1085:TYR:O	1:A:1087:PHE:N	1.97	0.96
1:A:607:ARG:HG2	1:A:611:ASP:OD2	1.64	0.96
1:A:365:SER:HA	1:A:662:LEU:CB	1.95	0.96
1:A:241:GLN:NE2	1:A:518:ARG:HH22	1.64	0.96
1:A:1156:ASN:HB3	1:A:1228:MET:HE1	1.47	0.96
1:A:1062:ALA:CB	1:A:1078:VAL:HB	1.95	0.96
1:A:591:VAL:CG1	1:A:603:PHE:CE1	2.49	0.96
1:A:653:LYS:O	1:A:682:LEU:HD21	1.65	0.96
1:A:659:ALA:O	1:A:662:LEU:HD23	1.66	0.96
1:A:684:LEU:HD21	1:A:728:LEU:HD22	1.40	0.95
1:A:923:ILE:O	1:A:1042:HIS:HB3	1.63	0.95
1:A:686:VAL:O	1:A:690:ILE:HG13	1.65	0.95
1:A:718:GLU:O	1:A:722:GLN:HB2	1.67	0.95
1:A:1062:ALA:CA	1:A:1078:VAL:HG21	1.95	0.95
1:A:879:ILE:O	1:A:1043:THR:CG2	2.14	0.95
1:A:1110:PHE:O	1:A:1114:MET:HG2	1.67	0.95
1:A:943:ILE:CB	1:A:1010:LYS:O	2.15	0.94
1:A:371:VAL:O	1:A:373:VAL:N	2.01	0.94
1:A:685:ILE:O	1:A:689:VAL:CG2	2.15	0.94
1:A:401:PRO:CG	1:A:571:TYR:CD1	2.49	0.94
1:A:720:LEU:O	1:A:723:GLN:NE2	1.98	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:680:LEU:CG	1:A:1229:TYR:OH	2.16	0.94
1:A:1055:LEU:HD23	1:A:1085:TYR:OH	1.66	0.94
1:A:656:LEU:CD1	1:A:685:ILE:HG12	1.93	0.94
1:A:1156:ASN:CG	1:A:1228:MET:HE3	1.92	0.94
1:A:724:LEU:CD2	1:A:1170:HIS:HE1	1.74	0.94
1:A:1046:GLN:CG	1:A:1050:ASP:OD2	2.16	0.94
1:A:398:HIS:HB3	1:A:399:PHE:CE1	2.02	0.94
1:A:591:VAL:HG11	1:A:603:PHE:CE1	2.02	0.93
1:A:692:PHE:CE1	1:A:713:GLU:HA	2.02	0.93
1:A:1135:LEU:HD21	1:A:1161:CYS:SG	2.08	0.93
1:A:635:ILE:CG2	1:A:690:ILE:HD11	1.98	0.93
1:A:635:ILE:CG2	1:A:690:ILE:HD13	1.94	0.93
1:A:752:SER:C	1:A:755:PRO:HD3	1.93	0.93
1:A:688:GLU:HG2	1:A:1170:HIS:CE1	2.03	0.93
1:A:1084:PHE:CZ	1:A:1085:TYR:CE1	2.57	0.93
1:A:729:GLY:O	1:A:733:PRO:CB	2.17	0.93
1:A:228:ASP:HB3	1:A:246:VAL:HG13	1.48	0.92
1:A:724:LEU:O	1:A:728:LEU:HG	1.70	0.92
1:A:507:ALA:HB1	1:A:529:LEU:CG	2.00	0.92
1:A:732:ALA:HB3	1:A:749:GLY:CA	1.98	0.92
1:A:1229:TYR:O	1:A:1233:VAL:HG23	1.69	0.92
1:A:241:GLN:HE22	1:A:518:ARG:NH2	1.68	0.92
1:A:401:PRO:HB2	1:A:569:ASN:HD21	1.30	0.92
1:A:678:ILE:HG12	1:A:748:LEU:HD21	1.51	0.92
1:A:1130:THR:HG21	1:A:1168:CYS:SG	2.08	0.92
1:A:1171:ILE:HG23	1:A:1191:LEU:CD2	2.00	0.92
1:A:1084:PHE:CZ	1:A:1085:TYR:HE1	1.87	0.92
1:A:401:PRO:HG3	1:A:571:TYR:HD1	1.01	0.92
1:A:879:ILE:O	1:A:1043:THR:HG22	1.71	0.91
1:A:135:ASN:HD22	5:A:1322:NAG:C1	1.66	0.91
1:A:1046:GLN:HG2	1:A:1050:ASP:OD2	1.71	0.91
1:A:680:LEU:HG	1:A:1229:TYR:OH	1.69	0.90
1:A:494:VAL:HA	1:A:497:HIS:CE1	2.06	0.90
1:A:620:ASP:O	1:A:623:THR:OG1	1.88	0.90
1:A:1156:ASN:CB	1:A:1228:MET:HE3	2.00	0.90
1:A:924:PHE:CB	1:A:1041:TYR:O	2.20	0.90
1:A:1141:VAL:O	1:A:1147:ILE:CB	2.19	0.90
1:A:1082:SER:O	1:A:1084:PHE:N	2.05	0.90
1:A:755:PRO:HD2	1:A:756:ALA:N	1.84	0.89
1:A:915:ASN:CB	1:A:920:VAL:CA	2.51	0.89
1:A:1059:ARG:HG3	1:A:1059:ARG:HH11	1.36	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1070:GLY:C	1:A:1071:ILE:HG13	1.96	0.89
1:A:396:ASP:O	1:A:400:GLY:N	2.04	0.89
1:A:929:LEU:CB	1:A:1038:PHE:HD2	1.81	0.89
1:A:228:ASP:HA	1:A:246:VAL:CG1	2.03	0.89
1:A:1098:THR:HG22	1:A:1154:LEU:CD2	2.03	0.89
1:A:659:ALA:HA	1:A:662:LEU:HD22	1.54	0.89
1:A:1133:MET:CG	1:A:1239:HIS:CE1	2.53	0.89
1:A:885:ALA:O	1:A:1079:PHE:O	1.89	0.89
1:A:1085:TYR:O	1:A:1088:TYR:N	2.06	0.89
1:A:641:HIS:O	1:A:642:MET:O	1.90	0.88
1:A:557:ASN:HD22	3:D:1:NAG:C1	1.79	0.88
1:A:1062:ALA:CB	1:A:1078:VAL:CB	2.52	0.88
1:A:632:PHE:HZ	1:A:650:VAL:HG23	1.39	0.88
1:A:693:LEU:HD11	1:A:763:PHE:HD2	1.36	0.88
1:A:1009:PRO:CA	1:A:1016:HIS:O	2.22	0.88
1:A:401:PRO:HD3	1:A:571:TYR:HE1	1.09	0.88
1:A:544:TRP:HD1	1:A:545:LEU:N	1.72	0.88
1:A:656:LEU:HB3	1:A:751:LEU:HD21	1.54	0.88
1:A:591:VAL:HG12	1:A:603:PHE:CZ	2.08	0.87
1:A:1082:SER:HB2	1:A:1084:PHE:CD1	2.08	0.87
1:A:1084:PHE:HE1	1:A:1085:TYR:CD1	1.88	0.87
1:A:680:LEU:HB3	1:A:1229:TYR:HH	1.37	0.87
1:A:1127:MET:CE	1:A:1168:CYS:CB	2.51	0.87
1:A:523:LEU:HD11	1:A:1016:HIS:CA	2.04	0.87
1:A:631:MET:HG3	1:A:1208:GLY:HA3	1.54	0.87
1:A:650:VAL:O	1:A:654:VAL:HG23	1.74	0.87
1:A:692:PHE:HZ	1:A:713:GLU:CB	1.86	0.87
1:A:692:PHE:CZ	1:A:713:GLU:HA	2.10	0.86
1:A:1138:MET:HE2	1:A:1232:MET:HB2	0.88	0.86
1:A:755:PRO:CD	1:A:756:ALA:H	1.88	0.86
1:A:384:PRO:HA	1:A:389:ARG:HG3	1.58	0.86
1:A:1133:MET:HE2	1:A:1239:HIS:CE1	2.09	0.85
1:A:459:ASN:HD22	5:A:1324:NAG:C1	1.87	0.85
1:A:507:ALA:CB	1:A:529:LEU:HG	2.05	0.85
1:A:856:VAL:O	1:A:1048:SER:HB2	1.75	0.85
1:A:631:MET:SD	1:A:1208:GLY:HA2	2.14	0.85
1:A:656:LEU:CB	1:A:682:LEU:CD1	2.53	0.85
1:A:684:LEU:HD11	1:A:728:LEU:CD2	2.06	0.85
1:A:879:ILE:HA	1:A:1043:THR:CG2	2.04	0.85
1:A:720:LEU:HD22	1:A:1170:HIS:CA	2.06	0.85
1:A:1178:SER:CB	1:A:1186:ARG:HD3	2.04	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:656:LEU:CD1	1:A:682:LEU:HD12	2.07	0.84
1:A:441:HIS:CE1	1:A:495:LEU:HD23	2.12	0.84
1:A:732:ALA:HB1	1:A:749:GLY:CA	2.02	0.84
1:A:926:ALA:O	1:A:1040:THR:CG2	2.23	0.84
1:A:894:GLU:CB	1:A:995:PHE:CB	2.55	0.84
1:A:402:PHE:O	1:A:403:PHE:CB	2.25	0.84
1:A:959:VAL:C	1:A:984:PRO:N	2.36	0.84
1:A:688:GLU:CG	1:A:1170:HIS:NE2	2.39	0.84
1:A:1127:MET:HE2	1:A:1168:CYS:CB	2.08	0.84
1:A:1156:ASN:HB3	1:A:1228:MET:HE3	1.60	0.83
1:A:228:ASP:CB	1:A:246:VAL:CG1	2.56	0.83
1:A:648:LEU:CB	1:A:763:PHE:CE1	2.60	0.83
1:A:196:LYS:CG	1:A:204:THR:OG1	2.25	0.83
1:A:401:PRO:HB2	1:A:569:ASN:CG	2.03	0.83
1:A:1133:MET:SD	1:A:1239:HIS:CE1	2.71	0.83
1:A:1167:PHE:CE2	1:A:1237:ALA:HA	2.12	0.83
1:A:167:SER:O	1:A:168:SER:OG	1.96	0.83
1:A:676:SER:OG	1:A:1226:PHE:HE2	1.60	0.82
1:A:687:ILE:O	1:A:691:PRO:CD	2.28	0.82
1:A:856:VAL:C	1:A:1048:SER:CB	2.53	0.82
1:A:1082:SER:HB2	1:A:1084:PHE:CE1	2.14	0.82
1:A:1229:TYR:CE1	1:A:1233:VAL:HG21	2.15	0.82
1:A:591:VAL:CG1	1:A:603:PHE:CZ	2.63	0.82
1:A:1055:LEU:HD22	1:A:1055:LEU:O	1.78	0.82
1:A:688:GLU:C	1:A:691:PRO:HD2	1.97	0.82
1:A:1140:GLY:O	1:A:1144:LEU:N	2.13	0.82
1:A:1156:ASN:CB	1:A:1228:MET:CE	2.57	0.82
1:A:1210:ILE:HG13	1:A:1214:ALA:HB3	1.61	0.82
1:A:631:MET:CG	1:A:1208:GLY:HA3	2.10	0.81
1:A:720:LEU:O	1:A:723:GLN:HG3	1.79	0.81
1:A:1209:GLY:HA3	1:A:1230:LEU:CD1	2.10	0.81
1:A:1209:GLY:O	1:A:1213:LEU:N	2.11	0.81
1:A:241:GLN:HE22	1:A:518:ARG:HH22	0.85	0.81
1:A:631:MET:CE	1:A:1204:LEU:C	2.44	0.81
1:A:1135:LEU:O	1:A:1139:PHE:HD2	1.64	0.81
1:A:684:LEU:HG	1:A:1166:GLU:HG3	1.61	0.81
1:A:1127:MET:HE2	1:A:1168:CYS:HB3	1.62	0.81
1:A:607:ARG:CG	1:A:611:ASP:CG	2.53	0.81
1:A:1171:ILE:CG2	1:A:1191:LEU:CD2	2.59	0.81
1:A:1068:THR:HG23	1:A:1069:MET:H	1.44	0.81
1:A:396:ASP:HA	1:A:400:GLY:CA	2.11	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1229:TYR:CD1	1:A:1233:VAL:HG21	2.15	0.80
1:A:228:ASP:HA	1:A:246:VAL:HG11	1.61	0.80
1:A:678:ILE:CG1	1:A:748:LEU:HD21	2.11	0.80
1:A:686:VAL:HG13	1:A:690:ILE:HD11	1.62	0.80
1:A:959:VAL:C	1:A:984:PRO:CB	2.54	0.80
1:A:985:GLU:CB	1:A:986:GLY:HA2	2.11	0.80
1:A:396:ASP:HA	1:A:400:GLY:HA2	1.64	0.80
1:A:404:ARG:HD2	1:A:567:VAL:CG2	2.12	0.80
1:A:633:LEU:O	1:A:636:SER:OG	1.99	0.80
1:A:656:LEU:HD13	1:A:685:ILE:HG12	1.56	0.80
1:A:684:LEU:CG	1:A:1166:GLU:HG3	2.10	0.80
1:A:628:TYR:OH	1:A:653:LYS:HD2	1.82	0.80
1:A:1142:MET:CE	1:A:1153:SER:OG	2.30	0.80
4:F:1:NAG:H62	4:F:2:NAG:HN2	1.47	0.80
3:D:1:NAG:H62	3:D:2:NAG:C8	2.12	0.79
1:A:381:TRP:HD1	1:A:382:SER:N	1.80	0.79
1:A:1142:MET:HE3	1:A:1148:SER:C	2.06	0.79
1:A:472:LEU:HD21	1:A:1017:ALA:CB	2.13	0.79
1:A:608:SER:O	1:A:612:GLU:HB2	1.82	0.79
1:A:337:ARG:HA	1:A:718:GLU:CG	2.12	0.79
1:A:730:GLU:HG2	1:A:1112:VAL:CG2	2.13	0.79
1:A:659:ALA:O	1:A:662:LEU:CD2	2.31	0.79
1:A:584:GLU:OE2	1:A:606:GLU:HB2	1.82	0.79
1:A:648:LEU:HD11	1:A:763:PHE:HA	1.63	0.79
1:A:1051:PHE:HB3	1:A:1084:PHE:HD2	1.49	0.79
1:A:1108:ALA:O	1:A:1112:VAL:CG2	2.28	0.78
1:A:1171:ILE:HG23	1:A:1191:LEU:HD23	1.63	0.78
1:A:1202:ILE:HG21	1:A:1237:ALA:HB1	1.62	0.78
1:A:185:ASN:HD22	5:A:1319:NAG:C1	1.93	0.78
1:A:720:LEU:CD2	1:A:1170:HIS:HA	2.11	0.78
1:A:401:PRO:CB	1:A:569:ASN:HD21	1.96	0.78
1:A:693:LEU:CD1	1:A:763:PHE:CD2	2.47	0.78
1:A:580:ALA:O	1:A:584:GLU:HG3	1.83	0.78
1:A:1142:MET:HE2	1:A:1153:SER:OG	1.84	0.78
1:A:629:ALA:O	1:A:633:LEU:HG	1.84	0.78
1:A:409:ILE:HG21	1:A:872:MET:CB	2.14	0.77
1:A:228:ASP:CA	1:A:246:VAL:HG13	2.14	0.77
1:A:653:LYS:C	1:A:653:LYS:HE3	2.09	0.77
1:A:688:GLU:OE1	1:A:721:ASP:OD1	2.02	0.77
1:A:632:PHE:CZ	1:A:650:VAL:HG23	2.19	0.77
1:A:1021:SER:O	1:A:1022:ALA:CB	2.32	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:693:LEU:HD12	1:A:763:PHE:CE2	2.01	0.77
1:A:1201:GLY:O	1:A:1205:THR:HG23	1.84	0.77
1:A:730:GLU:HG3	1:A:1108:ALA:HB1	0.87	0.77
1:A:879:ILE:C	1:A:1043:THR:HG21	2.00	0.77
1:A:648:LEU:HB3	1:A:763:PHE:CZ	2.17	0.77
1:A:407:GLN:HB3	1:A:604:THR:HG21	1.67	0.76
1:A:720:LEU:C	1:A:723:GLN:HE21	1.93	0.76
1:A:656:LEU:HD11	1:A:685:ILE:HG13	0.78	0.76
1:A:1194:MET:HA	1:A:1194:MET:CE	2.15	0.76
1:A:544:TRP:CD1	1:A:545:LEU:N	2.53	0.76
1:A:684:LEU:CD1	1:A:728:LEU:HD22	2.15	0.76
1:A:1110:PHE:HE2	1:A:1124:ALA:HB1	1.49	0.76
1:A:1135:LEU:O	1:A:1139:PHE:CD2	2.38	0.76
1:A:631:MET:CG	1:A:1208:GLY:CA	2.64	0.76
1:A:752:SER:HA	1:A:755:PRO:CG	2.15	0.76
1:A:726:ARG:HB3	1:A:1112:VAL:CG1	2.16	0.76
1:A:1184:VAL:O	1:A:1184:VAL:HG12	1.84	0.76
1:A:381:TRP:O	1:A:740:PHE:CB	2.33	0.75
1:A:1199:PHE:O	1:A:1203:THR:CG2	2.34	0.75
1:A:630:ILE:O	1:A:634:TYR:CD2	2.39	0.75
1:A:726:ARG:HB3	1:A:1112:VAL:HG11	1.68	0.75
1:A:403:PHE:HE2	1:A:566:PRO:HB3	0.94	0.75
1:A:494:VAL:HA	1:A:497:HIS:ND1	2.01	0.75
1:A:684:LEU:HD11	1:A:728:LEU:HD21	1.68	0.75
1:A:856:VAL:C	1:A:1048:SER:HB3	2.11	0.75
1:A:684:LEU:HD23	1:A:728:LEU:CD1	1.96	0.75
1:A:1114:MET:HE1	1:A:1124:ALA:HB2	1.67	0.75
1:A:676:SER:CB	1:A:1225:TYR:OH	2.30	0.75
1:A:631:MET:HE2	1:A:1204:LEU:O	1.81	0.74
1:A:720:LEU:HB3	1:A:1170:HIS:HD2	1.52	0.74
1:A:1138:MET:SD	1:A:1232:MET:HB2	2.26	0.74
1:A:621:VAL:O	1:A:625:VAL:HG23	1.87	0.74
1:A:1127:MET:CE	1:A:1130:THR:HG21	2.16	0.74
1:A:185:ASN:ND2	5:A:1319:NAG:O5	2.20	0.74
1:A:656:LEU:HD11	1:A:685:ILE:CG2	2.18	0.74
1:A:873:VAL:CB	1:A:1045:LEU:HD13	2.17	0.74
1:A:1062:ALA:HB2	1:A:1078:VAL:HG11	1.70	0.74
1:A:881:GLN:CB	1:A:1041:TYR:HB2	2.17	0.74
1:A:1045:LEU:CA	1:A:1051:PHE:CZ	2.71	0.74
1:A:441:HIS:NE2	1:A:496:ASP:OD1	2.21	0.74
1:A:396:ASP:CA	1:A:400:GLY:HA2	2.17	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1055:LEU:HD23	1:A:1085:TYR:CE2	2.23	0.73
3:D:1:NAG:C1	3:D:1:NAG:H82	2.18	0.73
1:A:250:LYS:HB3	1:A:251:PRO:HD2	1.68	0.73
1:A:515:TYR:CE1	1:A:526:THR:CG2	2.70	0.73
1:A:1068:THR:HG23	1:A:1069:MET:N	2.03	0.73
1:A:984:PRO:O	1:A:989:ARG:N	2.21	0.73
1:A:1046:GLN:O	1:A:1047:THR:OG1	2.06	0.73
1:A:684:LEU:HD11	1:A:1166:GLU:HG3	1.71	0.73
1:A:1045:LEU:CA	1:A:1051:PHE:HZ	2.00	0.73
1:A:228:ASP:CA	1:A:246:VAL:CG1	2.67	0.73
1:A:401:PRO:CB	1:A:569:ASN:OD1	2.36	0.73
1:A:1210:ILE:CD1	1:A:1214:ALA:HB2	2.19	0.73
1:A:368:LEU:O	1:A:665:LEU:CB	2.36	0.72
1:A:632:PHE:CZ	1:A:650:VAL:CG2	2.72	0.72
1:A:1127:MET:O	1:A:1130:THR:OG1	2.06	0.72
1:A:1062:ALA:HB1	1:A:1078:VAL:CG2	2.20	0.72
1:A:1211:VAL:O	1:A:1215:PHE:CB	2.38	0.72
1:A:158:ASN:CG	5:A:1303:NAG:C1	2.60	0.72
1:A:676:SER:HB3	1:A:1225:TYR:CZ	2.23	0.72
1:A:878:SER:C	1:A:1043:THR:HG21	2.13	0.72
1:A:1062:ALA:O	1:A:1066:THR:OG1	2.06	0.72
1:A:108:PHE:HE1	1:A:194:PHE:HE1	1.37	0.72
1:A:1138:MET:O	1:A:1142:MET:HG2	1.89	0.72
1:A:1084:PHE:CD1	1:A:1085:TYR:HD1	2.06	0.72
1:A:1203:THR:HG23	1:A:1204:LEU:N	2.03	0.71
1:A:1122:TRP:O	1:A:1126:ILE:HG13	1.89	0.71
1:A:1161:CYS:O	1:A:1165:VAL:HG23	1.91	0.71
3:D:1:NAG:C6	3:D:2:NAG:C8	2.68	0.71
1:A:259:PRO:O	1:A:260:TRP:CB	2.37	0.71
1:A:1131:ILE:O	1:A:1135:LEU:HG	1.90	0.71
1:A:929:LEU:CB	1:A:1038:PHE:HE2	1.98	0.71
1:A:404:ARG:HD2	1:A:567:VAL:HG23	1.72	0.71
1:A:1228:MET:HG3	1:A:1229:TYR:N	2.04	0.71
1:A:591:VAL:HB	1:A:603:PHE:HE1	1.55	0.71
1:A:915:ASN:HA	1:A:920:VAL:CA	2.17	0.71
1:A:544:TRP:CZ2	1:A:1041:TYR:HE1	2.07	0.71
1:A:689:VAL:HG21	1:A:759:THR:HG21	1.72	0.71
1:A:1051:PHE:HB3	1:A:1084:PHE:CD2	2.25	0.71
1:A:1124:ALA:O	1:A:1128:CYS:HB2	1.91	0.71
1:A:631:MET:SD	1:A:1208:GLY:HA3	2.30	0.70
1:A:751:LEU:C	1:A:751:LEU:HD23	2.15	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:754:MET:N	1:A:755:PRO:HD3	2.05	0.70
1:A:703:PHE:C	1:A:708:ALA:HB2	2.15	0.70
1:A:824:SER:CB	1:A:1188:GLU:OE1	2.40	0.70
1:A:1106:LEU:CD2	1:A:1131:ILE:HD13	2.22	0.70
1:A:1130:THR:CG2	1:A:1168:CYS:SG	2.79	0.70
1:A:1133:MET:HG2	1:A:1239:HIS:CG	2.24	0.70
1:A:386:SER:O	1:A:390:LEU:HD12	1.90	0.70
1:A:406:GLU:OE2	1:A:567:VAL:CG1	2.40	0.70
1:A:506:TYR:HB3	1:A:528:LEU:HD13	1.74	0.70
1:A:684:LEU:CD1	1:A:728:LEU:CD2	2.70	0.69
4:F:1:NAG:H62	4:F:2:NAG:N2	2.06	0.69
1:A:635:ILE:HG21	1:A:690:ILE:CD1	2.09	0.69
1:A:751:LEU:O	1:A:755:PRO:CD	2.41	0.69
1:A:730:GLU:HG2	1:A:1112:VAL:HG21	1.73	0.69
1:A:653:LYS:HB2	1:A:682:LEU:HD23	1.75	0.69
1:A:704:ILE:HA	1:A:708:ALA:HB3	1.75	0.69
4:F:2:NAG:H4	4:F:3:BMA:O2	1.93	0.69
1:A:524:ASN:HD22	2:C:1:NAG:C1	2.02	0.68
1:A:591:VAL:HB	1:A:603:PHE:CE1	2.27	0.68
1:A:1084:PHE:HZ	1:A:1085:TYR:HE1	1.38	0.68
1:A:692:PHE:CZ	1:A:713:GLU:CA	2.76	0.68
1:A:1046:GLN:HB3	1:A:1050:ASP:CG	2.18	0.68
1:A:656:LEU:CG	1:A:685:ILE:HG13	2.18	0.68
1:A:1203:THR:CG2	1:A:1204:LEU:N	2.55	0.68
1:A:752:SER:O	1:A:755:PRO:CG	2.41	0.68
1:A:1110:PHE:O	1:A:1114:MET:CG	2.39	0.68
1:A:656:LEU:HD13	1:A:682:LEU:HD12	1.75	0.68
1:A:722:GLN:HE21	1:A:1116:LEU:HD11	1.57	0.68
1:A:1047:THR:HG22	1:A:1048:SER:N	2.09	0.68
1:A:1065:VAL:O	1:A:1068:THR:CG2	2.36	0.68
1:A:544:TRP:CZ2	1:A:1041:TYR:CE1	2.82	0.68
1:A:692:PHE:HE1	1:A:713:GLU:HA	1.53	0.68
1:A:1110:PHE:CE2	1:A:1124:ALA:HB1	2.29	0.68
1:A:662:LEU:HG	1:A:663:ILE:N	2.07	0.67
1:A:1085:TYR:O	1:A:1086:VAL:C	2.37	0.67
1:A:1135:LEU:HB3	1:A:1139:PHE:HE2	1.59	0.67
1:A:1160:SER:HB2	1:A:1232:MET:SD	2.34	0.67
1:A:228:ASP:HA	1:A:246:VAL:HG13	1.74	0.67
1:A:407:GLN:HB3	1:A:604:THR:CG2	2.24	0.67
1:A:607:ARG:HG2	1:A:611:ASP:OD1	1.93	0.67
1:A:648:LEU:CD1	1:A:763:PHE:CD1	2.74	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:692:PHE:HZ	1:A:713:GLU:CA	2.08	0.67
1:A:762:LEU:O	1:A:766:LEU:HG	1.95	0.67
1:A:401:PRO:HB2	1:A:569:ASN:OD1	1.94	0.67
4:F:1:NAG:C6	4:F:2:NAG:C1	2.73	0.67
1:A:724:LEU:HD11	1:A:1166:GLU:HG2	0.84	0.67
1:A:1009:PRO:O	1:A:1010:LYS:O	2.11	0.67
1:A:1229:TYR:O	1:A:1233:VAL:CG2	2.43	0.67
1:A:704:ILE:HA	1:A:708:ALA:CB	2.24	0.67
1:A:755:PRO:CD	1:A:756:ALA:N	2.51	0.67
3:D:1:NAG:C6	3:D:2:NAG:H82	2.24	0.67
1:A:924:PHE:CA	1:A:925:ASN:CB	2.71	0.67
1:A:1098:THR:CG2	1:A:1154:LEU:HD21	2.13	0.67
1:A:685:ILE:HD13	1:A:685:ILE:N	2.09	0.67
1:A:1133:MET:CG	1:A:1239:HIS:CG	2.77	0.67
1:A:1080:PRO:HG2	1:A:1085:TYR:CE2	2.29	0.67
1:A:1062:ALA:HB2	1:A:1078:VAL:CG1	2.24	0.66
1:A:108:PHE:CE1	1:A:194:PHE:HE1	2.12	0.66
1:A:401:PRO:CD	1:A:571:TYR:HE1	1.96	0.66
1:A:950:VAL:O	1:A:951:LYS:CB	2.43	0.66
1:A:399:PHE:HE2	1:A:1022:ALA:HA	1.60	0.66
1:A:635:ILE:HG13	1:A:1204:LEU:HD13	1.77	0.66
1:A:691:PRO:HD2	1:A:692:PHE:H	1.60	0.66
1:A:1159:MET:HE1	1:A:1163:ILE:HD11	1.77	0.66
1:A:337:ARG:CA	1:A:718:GLU:HG3	2.23	0.66
1:A:630:ILE:HG22	1:A:634:TYR:HE2	1.59	0.66
1:A:1133:MET:HG3	1:A:1239:HIS:CD2	2.22	0.66
1:A:1213:LEU:C	1:A:1227:ARG:HH21	2.03	0.66
1:A:1022:ALA:O	1:A:1035:ALA:N	2.27	0.66
2:C:2:NAG:O7	2:C:2:NAG:O3	2.11	0.66
1:A:627:SER:OG	1:A:1212:VAL:CG2	2.43	0.66
1:A:757:VAL:O	1:A:760:PHE:HB2	1.96	0.66
1:A:916:ASN:N	1:A:919:LEU:O	2.23	0.66
1:A:656:LEU:HD12	1:A:682:LEU:HD12	1.77	0.66
1:A:1127:MET:HE1	1:A:1168:CYS:CB	2.19	0.66
1:A:1207:PHE:O	1:A:1210:ILE:HG22	1.96	0.66
1:A:1210:ILE:HG23	1:A:1211:VAL:N	2.11	0.66
1:A:690:ILE:O	1:A:694:VAL:HG23	1.96	0.65
1:A:1080:PRO:HG2	1:A:1085:TYR:HE2	1.61	0.65
1:A:472:LEU:HD22	1:A:538:GLY:HA3	1.78	0.65
1:A:627:SER:OG	1:A:1212:VAL:HG22	1.96	0.65
1:A:1046:GLN:CG	1:A:1050:ASP:CG	2.70	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1156:ASN:HD22	1:A:1228:MET:HE3	1.61	0.65
1:A:1114:MET:CE	1:A:1124:ALA:HB2	2.27	0.65
1:A:1133:MET:HE3	1:A:1239:HIS:HB2	1.79	0.65
1:A:688:GLU:CB	1:A:724:LEU:HD23	2.25	0.65
1:A:618:ASP:O	1:A:621:VAL:HG23	1.96	0.65
1:A:723:GLN:NE2	1:A:724:LEU:HB2	2.12	0.65
1:A:674:VAL:O	1:A:678:ILE:HG13	1.97	0.65
1:A:678:ILE:HG12	1:A:748:LEU:CD2	2.27	0.65
3:D:1:NAG:O6	3:D:2:NAG:C8	2.45	0.65
1:A:384:PRO:O	1:A:385:SER:OG	2.14	0.65
1:A:474:PRO:O	1:A:476:ASN:N	2.30	0.65
1:A:723:GLN:HG2	1:A:1173:ARG:HG3	1.79	0.64
1:A:395:PHE:CD2	1:A:1081:TYR:HD2	2.15	0.64
1:A:630:ILE:O	1:A:634:TYR:HD2	1.79	0.64
1:A:674:VAL:O	1:A:678:ILE:CD1	2.46	0.64
1:A:381:TRP:CD1	1:A:382:SER:N	2.64	0.64
1:A:591:VAL:CB	1:A:603:PHE:CE1	2.80	0.64
1:A:611:ASP:O	1:A:615:ARG:HB2	1.96	0.64
1:A:664:VAL:CG1	1:A:669:ALA:HB3	2.28	0.64
3:D:1:NAG:H62	3:D:2:NAG:H82	1.80	0.64
1:A:686:VAL:HG11	1:A:690:ILE:HD11	1.74	0.64
1:A:1082:SER:O	1:A:1084:PHE:HD1	1.79	0.64
1:A:396:ASP:C	1:A:400:GLY:H	2.06	0.64
1:A:640:GLY:O	1:A:642:MET:N	2.30	0.64
1:A:1167:PHE:CE2	1:A:1237:ALA:CA	2.79	0.64
1:A:653:LYS:HA	1:A:682:LEU:HG	1.80	0.64
1:A:684:LEU:HD21	1:A:728:LEU:HD11	1.69	0.64
1:A:684:LEU:HD22	1:A:728:LEU:HD22	1.75	0.64
1:A:407:GLN:O	1:A:604:THR:OG1	2.16	0.63
1:A:686:VAL:O	1:A:690:ILE:CG1	2.44	0.63
1:A:923:ILE:C	1:A:1042:HIS:CB	2.50	0.63
1:A:1062:ALA:CB	1:A:1078:VAL:HG11	2.29	0.63
1:A:423:TYR:CE1	1:A:424:PRO:HB3	2.33	0.63
1:A:607:ARG:O	1:A:611:ASP:HB2	1.99	0.63
1:A:879:ILE:O	1:A:1043:THR:HG21	1.92	0.63
1:A:1045:LEU:N	1:A:1051:PHE:CZ	2.67	0.63
1:A:252:GLN:O	1:A:254:PRO:HD3	1.99	0.63
1:A:692:PHE:CZ	1:A:713:GLU:CB	2.75	0.63
1:A:885:ALA:O	1:A:1079:PHE:HB2	1.99	0.63
1:A:1145:TRP:O	1:A:1147:ILE:N	2.31	0.63
1:A:403:PHE:HE2	1:A:566:PRO:CG	2.11	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1055:LEU:HD22	1:A:1055:LEU:C	2.24	0.63
1:A:1062:ALA:CB	1:A:1078:VAL:CG1	2.77	0.63
1:A:1137:ASN:HB3	1:A:1235:LEU:HD13	1.80	0.63
1:A:401:PRO:CG	1:A:571:TYR:CE1	2.79	0.63
1:A:686:VAL:O	1:A:690:ILE:N	2.30	0.63
1:A:630:ILE:HA	1:A:633:LEU:HD12	1.81	0.62
1:A:724:LEU:CD1	1:A:1166:GLU:HA	2.29	0.62
1:A:1138:MET:HE3	1:A:1138:MET:CA	2.22	0.62
1:A:1085:TYR:C	1:A:1087:PHE:N	2.57	0.62
1:A:751:LEU:C	1:A:755:PRO:HG3	2.20	0.62
1:A:752:SER:CA	1:A:755:PRO:CG	2.78	0.62
1:A:1171:ILE:HA	1:A:1194:MET:HG2	1.81	0.62
1:A:166:PRO:O	1:A:167:SER:OG	2.17	0.62
1:A:754:MET:N	1:A:755:PRO:CD	2.62	0.62
1:A:630:ILE:CG2	1:A:634:TYR:HE2	2.12	0.62
1:A:723:GLN:CD	1:A:1169:SER:HB2	2.17	0.62
1:A:732:ALA:HB3	1:A:749:GLY:HA2	1.82	0.62
1:A:252:GLN:C	1:A:254:PRO:HD3	2.25	0.62
1:A:1177:VAL:O	1:A:1186:ARG:NH1	2.32	0.62
1:A:875:TYR:O	1:A:876:PHE:O	2.18	0.62
1:A:1229:TYR:CD1	1:A:1233:VAL:CG2	2.82	0.62
1:A:1055:LEU:C	1:A:1055:LEU:HD13	2.25	0.61
1:A:401:PRO:HG3	1:A:571:TYR:CE1	2.29	0.61
1:A:228:ASP:HB2	1:A:246:VAL:CG1	2.29	0.61
1:A:622:PHE:O	1:A:626:ILE:HG13	2.01	0.61
1:A:1133:MET:CE	1:A:1239:HIS:CE1	2.74	0.61
1:A:1142:MET:HE1	1:A:1153:SER:OG	1.98	0.61
1:A:591:VAL:CB	1:A:603:PHE:HE1	2.12	0.61
1:A:631:MET:SD	1:A:1207:PHE:C	2.83	0.61
1:A:406:GLU:OE2	1:A:567:VAL:HG13	2.01	0.61
1:A:386:SER:O	1:A:390:LEU:HB2	2.01	0.61
1:A:680:LEU:O	1:A:683:THR:HG22	2.00	0.61
1:A:684:LEU:HD21	1:A:728:LEU:HD21	1.72	0.61
1:A:1199:PHE:O	1:A:1203:THR:HG22	2.00	0.61
1:A:1210:ILE:HG13	1:A:1214:ALA:CB	2.30	0.61
1:A:431:PHE:CE2	1:A:510:HIS:HD2	2.19	0.61
1:A:635:ILE:CG1	1:A:1204:LEU:HD13	2.31	0.61
1:A:1194:MET:O	1:A:1198:VAL:HG23	2.00	0.61
1:A:1021:SER:O	1:A:1022:ALA:HB3	2.01	0.61
1:A:631:MET:CE	1:A:1208:GLY:N	2.63	0.61
1:A:1092:LEU:HD13	1:A:1093:THR:N	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1186:ARG:HG3	1:A:1187:ALA:N	2.15	0.61
1:A:723:GLN:O	1:A:727:VAL:HG23	2.01	0.60
1:A:752:SER:HA	1:A:755:PRO:HG3	1.82	0.60
1:A:724:LEU:HD13	1:A:1166:GLU:HA	1.82	0.60
3:D:1:NAG:O6	3:D:2:NAG:H82	2.02	0.60
1:A:663:ILE:HD13	1:A:750:ALA:HB1	1.84	0.60
1:A:1046:GLN:HG2	1:A:1050:ASP:CG	2.25	0.60
1:A:1140:GLY:O	1:A:1144:LEU:CA	2.49	0.60
1:A:724:LEU:HD21	1:A:1166:GLU:CD	2.26	0.60
1:A:476:ASN:OD1	1:A:478:ASN:HB2	2.02	0.60
1:A:656:LEU:CD1	1:A:682:LEU:CD1	2.80	0.60
1:A:649:LEU:O	1:A:652:SER:N	2.35	0.60
1:A:882:TYR:CB	1:A:1082:SER:CB	2.64	0.60
1:A:1055:LEU:HD13	1:A:1056:LYS:N	2.17	0.60
1:A:764:ALA:O	1:A:768:VAL:HG23	2.02	0.60
1:A:373:VAL:O	1:A:375:THR:N	2.35	0.59
1:A:684:LEU:CD2	1:A:728:LEU:HD11	2.27	0.59
1:A:1209:GLY:O	1:A:1212:VAL:N	2.35	0.59
1:A:691:PRO:O	1:A:695:LEU:HG	2.02	0.59
1:A:752:SER:HA	1:A:755:PRO:HG2	1.84	0.59
1:A:1046:GLN:HB3	1:A:1050:ASP:CB	2.32	0.59
1:A:607:ARG:CG	1:A:611:ASP:OD1	2.50	0.59
1:A:924:PHE:CB	1:A:925:ASN:CA	2.80	0.59
1:A:122:ASN:ND2	1:A:217[B]:MET:CE	2.66	0.59
1:A:163:VAL:HA	1:A:242:ASP:O	2.01	0.59
1:A:881:GLN:CB	1:A:1041:TYR:CB	2.79	0.59
1:A:1080:PRO:HB2	1:A:1085:TYR:CZ	2.37	0.59
1:A:1138:MET:CE	1:A:1138:MET:HA	2.22	0.59
1:A:1229:TYR:HD1	1:A:1233:VAL:CG2	2.16	0.59
1:A:656:LEU:HA	1:A:751:LEU:HG	1.84	0.59
1:A:1106:LEU:HD23	1:A:1131:ILE:HD13	1.84	0.59
1:A:1091:TYR:HA	1:A:1094:ILE:CG1	2.31	0.59
1:A:1191:LEU:O	1:A:1195:GLY:N	2.36	0.59
1:A:382:SER:HB3	1:A:1086:VAL:O	2.03	0.59
1:A:732:ALA:CB	1:A:749:GLY:HA2	2.31	0.59
1:A:1142:MET:CE	1:A:1148:SER:C	2.71	0.59
1:A:1239:HIS:CE1	1:A:1243:PHE:CB	2.86	0.59
1:A:1149:LEU:HA	1:A:1153:SER:CB	2.33	0.59
1:A:985:GLU:HA	1:A:989:ARG:H	1.68	0.59
1:A:1071:ILE:C	1:A:1072:ASN:O	2.43	0.59
1:A:1133:MET:HE3	1:A:1239:HIS:CG	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:ALA:O	1:A:367:GLY:N	2.27	0.58
1:A:395:PHE:CD2	1:A:1081:TYR:CD2	2.91	0.58
1:A:637:LEU:HA	1:A:641:HIS:HA	1.84	0.58
1:A:648:LEU:CD1	1:A:763:PHE:HA	2.33	0.58
1:A:1070:GLY:O	1:A:1071:ILE:CB	2.50	0.58
1:A:1210:ILE:HD12	1:A:1214:ALA:HB2	1.84	0.58
1:A:648:LEU:HD12	1:A:763:PHE:HD1	1.65	0.58
1:A:1115:VAL:O	1:A:1115:VAL:HG12	2.02	0.58
1:A:733:PRO:C	1:A:735:MET:H	2.11	0.58
1:A:824:SER:CB	1:A:1188:GLU:CD	2.77	0.58
1:A:1112:VAL:HA	1:A:1115:VAL:HG23	1.85	0.58
1:A:752:SER:O	1:A:755:PRO:HG2	2.03	0.58
1:A:241:GLN:NE2	1:A:518:ARG:NH2	2.38	0.58
1:A:659:ALA:HA	1:A:662:LEU:HD21	1.71	0.58
1:A:1059:ARG:HH11	1:A:1059:ARG:CG	2.14	0.58
1:A:1084:PHE:CZ	1:A:1085:TYR:CD1	2.84	0.58
4:F:2:NAG:O3	4:F:3:BMA:H2	2.03	0.58
1:A:515:TYR:CE1	1:A:526:THR:HG23	2.38	0.58
1:A:656:LEU:HB3	1:A:751:LEU:CD2	2.31	0.57
1:A:250:LYS:CB	1:A:251:PRO:HD3	2.24	0.57
1:A:347:VAL:C	1:A:349:ASN:H	2.12	0.57
1:A:402:PHE:O	1:A:403:PHE:CD1	2.57	0.57
1:A:915:ASN:CB	1:A:919:LEU:C	2.77	0.57
1:A:1082:SER:CB	1:A:1084:PHE:CE1	2.86	0.57
1:A:664:VAL:HG13	1:A:669:ALA:HB3	1.85	0.57
1:A:688:GLU:O	1:A:691:PRO:CG	2.51	0.57
1:A:479:CYS:O	1:A:537:PHE:HB3	2.05	0.57
1:A:557:ASN:ND2	3:D:1:NAG:O5	2.38	0.57
1:A:1203:THR:CG2	1:A:1204:LEU:H	2.18	0.57
1:A:257:PRO:O	1:A:258:ALA:HB2	2.05	0.57
1:A:478:ASN:CG	4:F:1:NAG:C1	2.78	0.57
1:A:656:LEU:HD12	1:A:682:LEU:CD1	2.34	0.57
1:A:757:VAL:HA	1:A:760:PHE:HD2	1.70	0.57
1:A:720:LEU:O	1:A:723:GLN:CG	2.51	0.57
1:A:393:GLU:O	1:A:396:ASP:HB2	2.06	0.56
1:A:1062:ALA:CB	1:A:1078:VAL:CG2	2.82	0.56
1:A:252:GLN:H	1:A:253:PRO:HD3	1.70	0.56
1:A:1062:ALA:CB	1:A:1078:VAL:HG21	2.35	0.56
1:A:122:ASN:CG	1:A:217[B]:MET:HE1	2.29	0.56
1:A:635:ILE:HG22	1:A:649:LEU:HD11	1.86	0.56
1:A:676:SER:CB	1:A:1225:TYR:CZ	2.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:824:SER:HA	1:A:1188:GLU:CD	2.30	0.56
1:A:857:ASP:HA	1:A:1048:SER:HB3	1.87	0.56
1:A:1110:PHE:HD2	1:A:1128:CYS:HG	1.54	0.56
1:A:724:LEU:HD21	1:A:1170:HIS:HE1	1.66	0.56
1:A:924:PHE:CB	1:A:925:ASN:HA	2.36	0.56
3:D:1:NAG:C6	3:D:2:NAG:H83	2.36	0.56
1:A:396:ASP:HA	1:A:400:GLY:N	2.20	0.56
1:A:856:VAL:C	1:A:1048:SER:OG	2.49	0.56
1:A:1048:SER:HA	1:A:1088:TYR:CE2	2.41	0.56
1:A:723:GLN:HE22	1:A:724:LEU:HB2	1.71	0.56
1:A:752:SER:C	1:A:755:PRO:CG	2.78	0.56
1:A:441:HIS:CE1	1:A:496:ASP:OD1	2.59	0.56
1:A:1059:ARG:HG3	1:A:1059:ARG:NH1	2.09	0.56
1:A:371:VAL:C	1:A:373:VAL:N	2.64	0.56
1:A:655:SER:HB2	1:A:758:HIS:CD2	2.40	0.56
1:A:879:ILE:HA	1:A:1043:THR:HG23	1.85	0.56
1:A:1127:MET:HE1	1:A:1130:THR:HG21	1.87	0.56
1:A:191:GLU:OE2	1:A:195:ASN:ND2	2.39	0.56
1:A:1048:SER:O	1:A:1052:ILE:HD12	2.06	0.56
1:A:845:VAL:CB	1:A:1136:VAL:HG12	2.36	0.55
1:A:1106:LEU:HD22	1:A:1131:ILE:HD13	1.87	0.55
1:A:1117:LEU:CD2	1:A:1123:SER:HB3	2.36	0.55
1:A:1228:MET:HG3	1:A:1229:TYR:H	1.71	0.55
1:A:754:MET:O	1:A:757:VAL:HG22	2.07	0.55
1:A:398:HIS:CB	1:A:399:PHE:CE1	2.86	0.55
1:A:431:PHE:CZ	1:A:510:HIS:HD2	2.25	0.55
1:A:474:PRO:C	1:A:476:ASN:N	2.62	0.55
1:A:627:SER:O	1:A:631:MET:HG2	2.07	0.55
1:A:664:VAL:CG2	1:A:747:PHE:CB	2.85	0.55
3:D:1:NAG:H62	3:D:2:NAG:N2	2.21	0.55
1:A:92:GLN:HE22	1:A:526:THR:HB	1.71	0.55
1:A:1224:PHE:HA	1:A:1227:ARG:HB2	1.88	0.55
1:A:196:LYS:HG3	1:A:204:THR:HG1	1.64	0.55
1:A:491:SER:OG	1:A:494:VAL:HG23	2.06	0.55
1:A:1071:ILE:O	1:A:1072:ASN:C	2.46	0.55
1:A:1100:PHE:O	1:A:1104:VAL:HG23	2.07	0.55
1:A:407:GLN:O	1:A:604:THR:N	2.40	0.55
1:A:381:TRP:HD1	1:A:382:SER:H	1.55	0.55
1:A:444:LEU:HD23	1:A:492:HIS:CG	2.42	0.55
1:A:185:ASN:ND2	1:A:188:ASN:ND2	2.55	0.55
1:A:674:VAL:O	1:A:678:ILE:HD12	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:653:LYS:HG3	1:A:654:VAL:N	2.23	0.54
1:A:732:ALA:HB1	1:A:749:GLY:N	2.22	0.54
1:A:1202:ILE:HG21	1:A:1237:ALA:CB	2.34	0.54
1:A:762:LEU:O	1:A:766:LEU:CG	2.55	0.54
1:A:1055:LEU:CD2	1:A:1085:TYR:OH	2.47	0.54
1:A:1135:LEU:CD2	1:A:1161:CYS:SG	2.92	0.54
1:A:1239:HIS:O	1:A:1243:PHE:N	2.32	0.54
1:A:650:VAL:O	1:A:654:VAL:CG2	2.52	0.54
1:A:674:VAL:O	1:A:678:ILE:CG1	2.56	0.54
1:A:753:VAL:O	1:A:757:VAL:HG13	2.07	0.54
1:A:758:HIS:ND1	1:A:762:LEU:HD12	2.23	0.54
1:A:1229:TYR:HD1	1:A:1233:VAL:HG21	1.69	0.54
1:A:406:GLU:OE2	1:A:567:VAL:HG11	2.07	0.54
1:A:409:ILE:CG2	1:A:872:MET:CB	2.83	0.54
1:A:653:LYS:C	1:A:682:LEU:HD21	2.30	0.54
1:A:656:LEU:HD11	1:A:685:ILE:HG21	1.87	0.54
1:A:1137:ASN:HB3	1:A:1235:LEU:CD1	2.37	0.54
1:A:1167:PHE:CE2	1:A:1237:ALA:HB2	2.43	0.54
1:A:250:LYS:CB	1:A:251:PRO:CD	2.60	0.54
1:A:1062:ALA:C	1:A:1078:VAL:HG21	2.32	0.54
1:A:402:PHE:C	1:A:403:PHE:HD1	2.15	0.54
1:A:1133:MET:HG2	1:A:1239:HIS:HE2	1.51	0.54
1:A:1200:SER:O	1:A:1203:THR:HG22	2.07	0.54
1:A:252:GLN:N	1:A:253:PRO:HD3	2.22	0.54
1:A:398:HIS:C	1:A:399:PHE:CG	2.86	0.54
1:A:1092:LEU:C	1:A:1094:ILE:H	2.16	0.54
1:A:1109:ILE:O	1:A:1113:THR:HG23	2.07	0.54
1:A:691:PRO:CD	1:A:692:PHE:H	2.21	0.54
1:A:704:ILE:CA	1:A:708:ALA:HB3	2.38	0.54
1:A:1084:PHE:HE1	1:A:1085:TYR:CE1	2.08	0.54
1:A:1167:PHE:CE2	1:A:1237:ALA:CB	2.91	0.54
1:A:381:TRP:CD1	1:A:381:TRP:C	2.85	0.53
1:A:396:ASP:CB	1:A:400:GLY:HA2	2.38	0.53
1:A:398:HIS:HB3	1:A:399:PHE:CD1	2.42	0.53
1:A:684:LEU:CG	1:A:728:LEU:HD22	2.38	0.53
1:A:1133:MET:CE	1:A:1239:HIS:CB	2.86	0.53
1:A:1167:PHE:HE2	1:A:1237:ALA:CA	2.19	0.53
1:A:337:ARG:HA	1:A:718:GLU:CD	2.32	0.53
1:A:523:LEU:CD1	1:A:1016:HIS:N	2.71	0.53
1:A:649:LEU:HD22	1:A:686:VAL:HG13	1.90	0.53
4:F:1:NAG:H61	4:F:2:NAG:C1	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:ASN:ND2	1:A:217[B]:MET:HE1	2.23	0.53
1:A:1184:VAL:O	1:A:1184:VAL:CG1	2.53	0.53
1:A:93:PHE:CE1	1:A:175:LEU:HD13	2.44	0.53
1:A:371:VAL:C	1:A:373:VAL:H	2.08	0.53
1:A:1171:ILE:HG23	1:A:1191:LEU:HD22	1.90	0.53
1:A:402:PHE:C	1:A:403:PHE:CD1	2.87	0.53
1:A:686:VAL:HG12	1:A:690:ILE:CG1	2.34	0.53
1:A:632:PHE:HZ	1:A:650:VAL:CG2	2.11	0.53
1:A:1021:SER:O	1:A:1022:ALA:HB2	2.08	0.53
1:A:632:PHE:CZ	1:A:650:VAL:HG22	2.44	0.53
1:A:1234:LEU:O	1:A:1234:LEU:HD22	2.09	0.53
1:A:758:HIS:O	1:A:762:LEU:HB2	2.09	0.53
1:A:387:GLN:O	1:A:391:GLU:HB2	2.10	0.52
1:A:635:ILE:HG22	1:A:649:LEU:CD1	2.39	0.52
1:A:1234:LEU:O	1:A:1238:THR:HG23	2.09	0.52
1:A:861:ASP:CB	1:A:1219:GLN:CB	2.87	0.52
1:A:1081:TYR:C	1:A:1081:TYR:CD1	2.86	0.52
1:A:1202:ILE:O	1:A:1205:THR:OG1	2.21	0.52
1:A:688:GLU:HA	1:A:691:PRO:HG3	1.91	0.52
1:A:924:PHE:CB	1:A:925:ASN:CB	2.87	0.52
1:A:164:GLU:OE1	1:A:241:GLN:O	2.26	0.52
1:A:724:LEU:O	1:A:728:LEU:CG	2.53	0.52
1:A:1120:GLU:O	1:A:1124:ALA:HB3	2.10	0.52
1:A:1239:HIS:NE2	1:A:1243:PHE:CB	2.73	0.52
1:A:685:ILE:O	1:A:689:VAL:CB	2.57	0.52
1:A:915:ASN:CB	1:A:920:VAL:N	2.73	0.52
1:A:1047:THR:HG22	1:A:1048:SER:H	1.75	0.52
1:A:402:PHE:O	1:A:403:PHE:CG	2.63	0.52
1:A:474:PRO:C	1:A:476:ASN:H	2.18	0.52
1:A:631:MET:CG	1:A:1208:GLY:HA2	2.36	0.52
1:A:1068:THR:CG2	1:A:1069:MET:N	2.73	0.52
1:A:1210:ILE:CG2	1:A:1211:VAL:N	2.73	0.52
1:A:656:LEU:HB3	1:A:751:LEU:HD11	1.91	0.52
1:A:690:ILE:N	1:A:691:PRO:CD	2.73	0.52
1:A:1063:SER:O	1:A:1067:GLU:HB2	2.10	0.52
1:A:1210:ILE:O	1:A:1214:ALA:N	2.43	0.52
1:A:377:PRO:CB	1:A:378:VAL:HA	2.39	0.51
1:A:1091:TYR:HA	1:A:1094:ILE:HG13	1.90	0.51
1:A:1138:MET:SD	1:A:1138:MET:N	2.83	0.51
1:A:1167:PHE:HE2	1:A:1237:ALA:HB2	1.74	0.51
1:A:1193:HIS:O	1:A:1194:MET:HE3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:627:SER:CB	1:A:1211:VAL:HB	2.40	0.51
1:A:683:THR:HG23	1:A:684:LEU:N	2.25	0.51
1:A:758:HIS:C	1:A:760:PHE:H	2.18	0.51
1:A:915:ASN:CB	1:A:919:LEU:O	2.59	0.51
1:A:1047:THR:CG2	1:A:1048:SER:N	2.73	0.51
1:A:1068:THR:CG2	1:A:1069:MET:H	2.17	0.51
1:A:584:GLU:OE2	1:A:606:GLU:CB	2.56	0.51
1:A:1044:VAL:HB	1:A:1051:PHE:CE1	2.45	0.51
1:A:723:GLN:NE2	1:A:724:LEU:N	2.59	0.51
1:A:751:LEU:O	1:A:751:LEU:HD23	2.11	0.51
1:A:1080:PRO:HB2	1:A:1085:TYR:OH	2.10	0.51
1:A:1119:CYS:CB	1:A:1122:TRP:CB	2.89	0.51
1:A:401:PRO:CB	1:A:569:ASN:ND2	2.58	0.51
1:A:1084:PHE:CD1	1:A:1085:TYR:N	2.78	0.51
1:A:885:ALA:O	1:A:1079:PHE:C	2.53	0.51
1:A:1210:ILE:HG23	1:A:1211:VAL:H	1.76	0.51
1:A:724:LEU:HD23	1:A:1170:HIS:NE2	2.17	0.51
1:A:1115:VAL:C	1:A:1116:LEU:HG	2.36	0.51
1:A:1209:GLY:CA	1:A:1230:LEU:HD13	2.30	0.51
1:A:523:LEU:CD1	1:A:1015:GLY:C	2.83	0.51
1:A:544:TRP:HZ2	1:A:1041:TYR:CE1	2.26	0.51
1:A:923:ILE:CA	1:A:1042:HIS:HB3	2.41	0.51
1:A:523:LEU:HD11	1:A:1016:HIS:N	2.26	0.50
1:A:695:LEU:HD11	1:A:1194:MET:HE1	1.92	0.50
1:A:1121:LEU:O	1:A:1125:VAL:HB	2.11	0.50
1:A:114:SER:O	1:A:117:GLN:HG3	2.11	0.50
1:A:1133:MET:CE	1:A:1239:HIS:HB2	2.41	0.50
1:A:423:TYR:CZ	1:A:424:PRO:HB3	2.46	0.50
1:A:611:ASP:O	1:A:615:ARG:CB	2.60	0.50
1:A:676:SER:OG	1:A:1225:TYR:CE1	2.64	0.50
1:A:959:VAL:CA	1:A:984:PRO:N	2.74	0.50
1:A:1133:MET:HE3	1:A:1239:HIS:CB	2.41	0.50
1:A:1153:SER:HA	1:A:1156:ASN:HB2	1.94	0.50
1:A:1229:TYR:HE1	1:A:1233:VAL:HG21	1.70	0.50
1:A:167:SER:C	1:A:168:SER:HG	2.10	0.50
1:A:749:GLY:O	1:A:752:SER:CB	2.60	0.50
1:A:384:PRO:HA	1:A:389:ARG:CG	2.38	0.50
1:A:403:PHE:CD2	1:A:566:PRO:CB	2.77	0.50
1:A:515:TYR:CE1	1:A:526:THR:HG22	2.45	0.50
1:A:1111:LEU:O	1:A:1115:VAL:HG23	2.11	0.50
1:A:663:ILE:HD11	1:A:754:MET:HG3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1167:PHE:CD2	1:A:1237:ALA:HA	2.47	0.50
1:A:656:LEU:CA	1:A:751:LEU:HG	2.41	0.50
1:A:659:ALA:O	1:A:663:ILE:HG13	2.12	0.50
1:A:719:THR:O	1:A:723:GLN:HG3	2.12	0.50
1:A:753:VAL:C	1:A:755:PRO:CD	2.85	0.50
1:A:1090:GLN:C	1:A:1092:LEU:H	2.19	0.50
1:A:726:ARG:HB3	1:A:1112:VAL:HG13	1.93	0.49
1:A:1115:VAL:O	1:A:1116:LEU:HG	2.12	0.49
1:A:381:TRP:C	1:A:383:ALA:H	2.19	0.49
1:A:686:VAL:CG1	1:A:690:ILE:CG1	2.90	0.49
1:A:122:ASN:CG	1:A:217[B]:MET:CE	2.85	0.49
1:A:399:PHE:CE2	1:A:1022:ALA:HA	2.45	0.49
1:A:1152:VAL:HG11	1:A:1225:TYR:HD2	1.76	0.49
1:A:1223:ILE:O	1:A:1227:ARG:CG	2.61	0.49
1:A:423:TYR:CG	1:A:424:PRO:HA	2.47	0.49
1:A:627:SER:HB3	1:A:1211:VAL:HB	1.93	0.49
1:A:631:MET:CE	1:A:1208:GLY:H	2.26	0.49
1:A:729:GLY:O	1:A:733:PRO:N	2.45	0.49
1:A:1117:LEU:HD13	1:A:1173:ARG:HD3	1.93	0.49
1:A:1223:ILE:O	1:A:1227:ARG:HG2	2.11	0.49
3:D:1:NAG:O6	3:D:2:NAG:H83	2.12	0.49
1:A:344:SER:O	1:A:348:ARG:N	2.41	0.49
1:A:641:HIS:C	1:A:642:MET:O	2.55	0.49
1:A:713:GLU:C	1:A:715:LEU:H	2.20	0.49
1:A:720:LEU:C	1:A:723:GLN:HG3	2.37	0.49
1:A:35:TYR:CZ	1:A:38:LYS:HD2	2.48	0.49
1:A:431:PHE:CZ	1:A:510:HIS:CD2	3.00	0.48
1:A:618:ASP:O	1:A:621:VAL:CG2	2.60	0.48
1:A:1091:TYR:HA	1:A:1094:ILE:HG12	1.94	0.48
1:A:1130:THR:HA	1:A:1133:MET:HB3	1.95	0.48
1:A:656:LEU:HB3	1:A:682:LEU:CD1	2.42	0.48
1:A:885:ALA:O	1:A:1079:PHE:CA	2.61	0.48
1:A:382:SER:HA	1:A:1090:GLN:HG3	1.93	0.48
1:A:985:GLU:CB	1:A:989:ARG:CB	2.91	0.48
1:A:1159:MET:HE1	1:A:1163:ILE:CD1	2.43	0.48
1:A:720:LEU:HD21	1:A:1170:HIS:O	2.14	0.48
1:A:228:ASP:CG	1:A:245:ILE:HG21	2.39	0.48
1:A:1093:THR:O	1:A:1093:THR:HG22	2.13	0.48
1:A:1178:SER:CB	1:A:1186:ARG:CZ	2.89	0.48
1:A:382:SER:O	1:A:383:ALA:HB3	2.12	0.48
1:A:421:GLN:HB3	1:A:426:GLY:HA2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:444:LEU:HD23	1:A:492:HIS:CE1	2.49	0.48
1:A:544:TRP:O	1:A:879:ILE:CB	2.62	0.48
1:A:1044:VAL:O	1:A:1045:LEU:C	2.56	0.48
1:A:168:SER:C	1:A:170:ASP:H	2.20	0.48
1:A:598:ASN:ND2	2:E:1:NAG:C2	2.70	0.48
1:A:404:ARG:HG3	1:A:567:VAL:O	2.13	0.48
1:A:1060:LEU:O	1:A:1063:SER:OG	2.25	0.48
1:A:472:LEU:HB3	1:A:476:ASN:HB3	1.96	0.47
1:A:637:LEU:O	1:A:638:ALA:C	2.57	0.47
1:A:648:LEU:CB	1:A:763:PHE:CZ	2.93	0.47
1:A:690:ILE:O	1:A:690:ILE:HG22	2.14	0.47
1:A:878:SER:C	1:A:1043:THR:CG2	2.86	0.47
1:A:1071:ILE:CG2	1:A:1072:ASN:N	2.34	0.47
1:A:108:PHE:HE1	1:A:194:PHE:CE1	2.26	0.47
1:A:352:CYS:O	1:A:353:VAL:C	2.56	0.47
1:A:684:LEU:HG	1:A:1166:GLU:CG	2.38	0.47
1:A:704:ILE:CA	1:A:708:ALA:CB	2.92	0.47
1:A:252:GLN:N	1:A:253:PRO:CD	2.78	0.47
1:A:616:GLU:O	1:A:618:ASP:N	2.48	0.47
1:A:880:SER:O	1:A:1043:THR:HG22	2.15	0.47
1:A:893:LEU:O	1:A:894:GLU:C	2.55	0.47
1:A:421:GLN:H	1:A:421:GLN:CD	2.20	0.47
1:A:911:GLY:C	1:A:913:GLY:H	2.22	0.47
1:A:915:ASN:HA	1:A:921:GLN:N	2.29	0.47
1:A:653:LYS:O	1:A:653:LYS:HE3	2.13	0.47
1:A:656:LEU:CD2	1:A:685:ILE:HG13	2.45	0.47
1:A:673:GLY:C	1:A:675:PHE:H	2.23	0.47
1:A:684:LEU:CD2	1:A:728:LEU:CG	2.57	0.47
1:A:1063:SER:O	1:A:1067:GLU:CB	2.62	0.47
1:A:1063:SER:O	1:A:1067:GLU:HG3	2.14	0.47
1:A:1085:TYR:C	1:A:1087:PHE:H	2.22	0.47
1:A:1149:LEU:HA	1:A:1153:SER:HB2	1.97	0.47
1:A:1210:ILE:CD1	1:A:1214:ALA:CB	2.91	0.47
1:A:1229:TYR:CD1	1:A:1229:TYR:C	2.93	0.47
1:A:598:ASN:CG	2:E:1:NAG:C1	2.77	0.47
1:A:688:GLU:HB2	1:A:724:LEU:CD2	2.44	0.47
1:A:1059:ARG:CG	1:A:1059:ARG:NH1	2.73	0.47
1:A:1062:ALA:O	1:A:1078:VAL:HG21	2.15	0.47
1:A:437:ILE:HD13	1:A:509:TYR:CD1	2.50	0.47
1:A:985:GLU:CB	1:A:986:GLY:CA	2.87	0.47
1:A:38:LYS:HB3	1:A:202:PRO:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:635:ILE:HG21	1:A:686:VAL:HG11	1.97	0.47
1:A:688:GLU:HA	1:A:691:PRO:CG	2.45	0.47
1:A:733:PRO:C	1:A:735:MET:N	2.73	0.47
1:A:196:LYS:HE2	1:A:196:LYS:HB2	1.68	0.46
1:A:372:ARG:C	1:A:374:THR:H	2.23	0.46
1:A:544:TRP:CD1	1:A:544:TRP:C	2.92	0.46
1:A:635:ILE:HG12	1:A:1204:LEU:CD1	2.44	0.46
1:A:656:LEU:CB	1:A:751:LEU:HD11	2.45	0.46
1:A:659:ALA:C	1:A:662:LEU:CD2	2.63	0.46
1:A:1232:MET:HG3	1:A:1233:VAL:N	2.29	0.46
1:A:648:LEU:CG	1:A:763:PHE:CD1	2.98	0.46
3:D:1:NAG:C1	3:D:1:NAG:C8	2.86	0.46
1:A:544:TRP:CD1	1:A:545:LEU:H	2.30	0.46
1:A:649:LEU:O	1:A:650:VAL:C	2.57	0.46
1:A:736:PHE:O	1:A:737:LEU:O	2.33	0.46
1:A:824:SER:HA	1:A:1188:GLU:OE2	2.16	0.46
1:A:1045:LEU:HD23	1:A:1051:PHE:HZ	1.79	0.46
1:A:396:ASP:HA	1:A:400:GLY:H	1.80	0.46
1:A:758:HIS:C	1:A:760:PHE:N	2.74	0.46
1:A:476:ASN:HA	4:F:1:NAG:H82	1.97	0.46
1:A:632:PHE:HE1	1:A:649:LEU:CB	2.28	0.46
1:A:1167:PHE:HE2	1:A:1237:ALA:CB	2.27	0.46
1:A:515:TYR:HE1	1:A:526:THR:CG2	2.28	0.46
1:A:704:ILE:N	1:A:708:ALA:HB2	2.29	0.46
1:A:656:LEU:HD22	1:A:751:LEU:CD2	2.46	0.46
1:A:1009:PRO:C	1:A:1010:LYS:O	2.59	0.46
1:A:1220:ILE:O	1:A:1221:PHE:C	2.59	0.46
1:A:1228:MET:O	1:A:1229:TYR:C	2.58	0.46
1:A:401:PRO:CG	1:A:569:ASN:OD1	2.64	0.46
1:A:472:LEU:HD21	1:A:1017:ALA:HB1	1.96	0.46
1:A:1082:SER:C	1:A:1084:PHE:N	2.74	0.46
1:A:1222:GLN:C	1:A:1224:PHE:N	2.72	0.46
1:A:1229:TYR:HD1	1:A:1229:TYR:C	2.24	0.46
1:A:985:GLU:HA	1:A:989:ARG:CB	2.46	0.46
1:A:1048:SER:O	1:A:1052:ILE:CD1	2.63	0.46
1:A:687:ILE:C	1:A:691:PRO:HD3	2.35	0.45
1:A:381:TRP:C	1:A:383:ALA:N	2.74	0.45
1:A:484:VAL:HG11	1:A:547:LEU:HD21	1.98	0.45
1:A:1065:VAL:C	1:A:1068:THR:HG22	2.36	0.45
6:A:1325:CLR:H272	6:A:1325:CLR:H232	1.79	0.45
1:A:165:ALA:O	1:A:167:SER:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:627:SER:CB	1:A:1212:VAL:HG23	2.47	0.45
1:A:1127:MET:HE3	1:A:1130:THR:CG2	2.46	0.45
1:A:1166:GLU:O	1:A:1169:SER:OG	2.29	0.45
1:A:688:GLU:CB	1:A:724:LEU:CD2	2.89	0.45
1:A:1210:ILE:CG2	1:A:1211:VAL:H	2.29	0.45
1:A:162:ASP:OD2	1:A:244:SER:OG	2.32	0.45
1:A:91:LEU:HD13	1:A:101:PHE:CZ	2.52	0.45
1:A:635:ILE:HG21	1:A:686:VAL:CG1	2.46	0.45
1:A:649:LEU:CD2	1:A:686:VAL:HG13	2.47	0.45
1:A:659:ALA:CA	1:A:662:LEU:HD21	2.36	0.45
1:A:676:SER:CB	1:A:1225:TYR:CE1	2.99	0.45
1:A:1154:LEU:HD23	1:A:1154:LEU:HA	1.78	0.45
1:A:398:HIS:C	1:A:399:PHE:CD1	2.95	0.45
1:A:684:LEU:CG	1:A:728:LEU:CD2	2.95	0.45
1:A:688:GLU:CA	1:A:691:PRO:HD3	2.45	0.45
1:A:1140:GLY:C	1:A:1144:LEU:CB	2.83	0.45
1:A:1225:TYR:HD1	1:A:1226:PHE:CG	2.35	0.45
1:A:1194:MET:HE3	1:A:1194:MET:CA	2.28	0.44
1:A:1080:PRO:O	1:A:1085:TYR:CE2	2.70	0.44
1:A:135:ASN:ND2	5:A:1322:NAG:O5	2.21	0.44
1:A:404:ARG:HH11	1:A:404:ARG:CG	2.30	0.44
1:A:1138:MET:CE	1:A:1138:MET:CA	2.91	0.44
1:A:396:ASP:O	1:A:399:PHE:N	2.50	0.44
1:A:690:ILE:N	1:A:691:PRO:HD3	2.32	0.44
1:A:875:TYR:C	1:A:876:PHE:O	2.60	0.44
1:A:1053:ASP:O	1:A:1057:LYS:HD2	2.18	0.44
1:A:27:TRP:NE1	1:A:117:GLN:HE22	2.16	0.44
1:A:238:CYS:O	1:A:246:VAL:HG21	2.17	0.44
1:A:382:SER:OG	1:A:1086:VAL:HG13	2.17	0.44
1:A:1043:THR:C	1:A:1044:VAL:HG23	2.42	0.44
1:A:720:LEU:O	1:A:723:GLN:CD	2.60	0.44
1:A:723:GLN:OE1	1:A:1169:SER:CA	2.63	0.44
1:A:1127:MET:CE	1:A:1130:THR:CG2	2.92	0.44
1:A:66:PHE:HB3	1:A:73:LEU:HD21	2.00	0.44
1:A:396:ASP:CA	1:A:400:GLY:H	2.30	0.44
1:A:688:GLU:HB2	1:A:724:LEU:HD21	1.98	0.44
1:A:246:VAL:HG23	1:A:246:VAL:O	2.18	0.44
1:A:683:THR:CG2	1:A:684:LEU:N	2.80	0.44
1:A:691:PRO:HB3	1:A:1197:SER:HB2	2.00	0.44
1:A:885:ALA:O	1:A:1079:PHE:CB	2.65	0.44
1:A:1048:SER:O	1:A:1052:ILE:HG13	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1117:LEU:HD23	1:A:1123:SER:HB3	2.00	0.44
1:A:444:LEU:HD23	1:A:492:HIS:CD2	2.53	0.43
1:A:653:LYS:HG3	1:A:654:VAL:H	1.82	0.43
1:A:1047:THR:CG2	1:A:1048:SER:H	2.30	0.43
1:A:1133:MET:SD	1:A:1239:HIS:ND1	2.78	0.43
1:A:474:PRO:O	1:A:475:TYR:C	2.60	0.43
1:A:732:ALA:O	1:A:746:PHE:HA	2.17	0.43
1:A:734:SER:C	1:A:736:PHE:H	2.25	0.43
1:A:1094:ILE:O	1:A:1098:THR:HG23	2.18	0.43
1:A:1156:ASN:ND2	1:A:1228:MET:CE	2.68	0.43
1:A:1198:VAL:O	1:A:1202:ILE:HB	2.19	0.43
1:A:421:GLN:CD	1:A:421:GLN:N	2.77	0.43
1:A:749:GLY:O	1:A:752:SER:HB2	2.18	0.43
1:A:632:PHE:HE1	1:A:649:LEU:HB3	1.83	0.43
1:A:1041:TYR:CD1	1:A:1041:TYR:N	2.86	0.43
1:A:1090:GLN:O	1:A:1094:ILE:HG12	2.19	0.43
1:A:1092:LEU:HD13	1:A:1092:LEU:C	2.44	0.43
1:A:364:CYS:O	1:A:662:LEU:HB2	2.18	0.43
1:A:1202:ILE:O	1:A:1203:THR:C	2.61	0.43
1:A:1222:GLN:C	1:A:1224:PHE:H	2.26	0.43
1:A:653:LYS:HA	1:A:682:LEU:CG	2.47	0.43
1:A:690:ILE:O	1:A:694:VAL:CG2	2.64	0.43
1:A:750:ALA:C	1:A:752:SER:N	2.75	0.43
1:A:930:ASP:O	1:A:933:THR:N	2.50	0.43
1:A:1100:PHE:CE1	1:A:1104:VAL:CG2	3.02	0.43
1:A:239:SER:O	1:A:243:CYS:HB3	2.19	0.42
1:A:607:ARG:C	1:A:611:ASP:HB2	2.43	0.42
1:A:627:SER:CB	1:A:1212:VAL:CG2	2.96	0.42
1:A:653:LYS:C	1:A:653:LYS:CE	2.86	0.42
1:A:1141:VAL:C	1:A:1147:ILE:CB	2.89	0.42
1:A:386:SER:O	1:A:390:LEU:CD1	2.65	0.42
1:A:637:LEU:O	1:A:638:ALA:O	2.37	0.42
1:A:767:ALA:O	1:A:771:ASP:N	2.52	0.42
1:A:1063:SER:O	1:A:1067:GLU:CG	2.67	0.42
1:A:523:LEU:CG	1:A:1016:HIS:CB	2.96	0.42
1:A:1160:SER:HB2	1:A:1232:MET:CE	2.50	0.42
1:A:622:PHE:O	1:A:626:ILE:CG1	2.67	0.42
1:A:1093:THR:HG22	1:A:1096:ASP:HB2	2.01	0.42
1:A:723:GLN:HG2	1:A:1173:ARG:CG	2.46	0.42
1:A:726:ARG:NE	1:A:726:ARG:HA	2.35	0.42
1:A:1117:LEU:HB3	1:A:1118:GLY:H	1.70	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1199:PHE:O	1:A:1203:THR:HB	2.20	0.42
1:A:196:LYS:HG3	1:A:196:LYS:H	1.53	0.42
1:A:404:ARG:HH11	1:A:404:ARG:CB	2.32	0.42
1:A:507:ALA:CB	1:A:529:LEU:CG	2.80	0.42
1:A:509:TYR:CZ	1:A:510:HIS:CE1	3.08	0.42
1:A:656:LEU:CD2	1:A:751:LEU:O	2.67	0.42
1:A:668:VAL:O	1:A:669:ALA:HB2	2.20	0.42
1:A:685:ILE:O	1:A:689:VAL:HB	2.19	0.42
1:A:942:TRP:O	1:A:943:ILE:CB	2.68	0.42
1:A:1090:GLN:C	1:A:1092:LEU:N	2.76	0.42
1:A:1173:ARG:HA	1:A:1173:ARG:HD2	1.75	0.42
1:A:1235:LEU:O	1:A:1238:THR:OG1	2.37	0.42
1:A:1045:LEU:HD23	1:A:1051:PHE:CZ	2.54	0.42
1:A:370:PHE:O	1:A:371:VAL:CB	2.67	0.42
1:A:686:VAL:HG13	1:A:690:ILE:CD1	2.34	0.42
1:A:691:PRO:CD	1:A:692:PHE:N	2.83	0.42
1:A:399:PHE:CD1	1:A:399:PHE:N	2.88	0.42
1:A:423:TYR:HA	1:A:424:PRO:HA	1.79	0.42
1:A:635:ILE:HG12	1:A:1204:LEU:HD12	2.02	0.42
1:A:653:LYS:HA	1:A:682:LEU:CD2	2.50	0.42
1:A:656:LEU:CD1	1:A:685:ILE:CB	2.62	0.42
1:A:202:PRO:HG2	1:A:203:PHE:CE2	2.55	0.41
1:A:908:VAL:HG13	1:A:926:ALA:HA	2.02	0.41
1:A:1131:ILE:O	1:A:1135:LEU:CG	2.63	0.41
1:A:1202:ILE:CG2	1:A:1237:ALA:CB	2.98	0.41
1:A:1227:ARG:HA	1:A:1227:ARG:HD3	1.78	0.41
1:A:635:ILE:CG1	1:A:1204:LEU:CD1	2.98	0.41
1:A:648:LEU:O	1:A:649:LEU:C	2.62	0.41
1:A:673:GLY:C	1:A:675:PHE:N	2.78	0.41
1:A:726:ARG:CB	1:A:1112:VAL:CG1	2.95	0.41
1:A:893:LEU:O	1:A:895:GLU:N	2.53	0.41
1:A:1171:ILE:CG2	1:A:1191:LEU:HD21	2.47	0.41
3:D:2:NAG:H62	3:D:3:BMA:C1	2.48	0.41
1:A:726:ARG:CB	1:A:1112:VAL:HG11	2.45	0.41
1:A:730:GLU:HG2	1:A:1112:VAL:HG23	1.99	0.41
1:A:1058:ALA:HA	1:A:1061:ILE:HD12	2.03	0.41
1:A:680:LEU:O	1:A:683:THR:CG2	2.68	0.41
1:A:876:PHE:O	1:A:877:LYS:CB	2.67	0.41
1:A:1117:LEU:HD11	1:A:1173:ARG:HH11	1.84	0.41
1:A:1207:PHE:HD1	1:A:1207:PHE:HA	1.78	0.41
1:A:507:ALA:CB	1:A:529:LEU:CD2	2.98	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:684:LEU:HD11	1:A:1166:GLU:CG	2.47	0.41
1:A:1152:VAL:O	1:A:1155:VAL:N	2.54	0.41
1:A:1225:TYR:HD1	1:A:1226:PHE:CD1	2.39	0.41
1:A:347:VAL:C	1:A:349:ASN:N	2.78	0.41
1:A:384:PRO:C	1:A:385:SER:HG	2.20	0.41
1:A:1199:PHE:O	1:A:1203:THR:HG21	2.19	0.41
1:A:639:LEU:C	1:A:641:HIS:N	2.79	0.41
1:A:751:LEU:O	1:A:755:PRO:HD3	2.17	0.41
1:A:824:SER:CA	1:A:1188:GLU:CD	2.93	0.41
1:A:885:ALA:O	1:A:1079:PHE:N	2.54	0.41
1:A:1127:MET:HE2	1:A:1168:CYS:HB2	1.98	0.41
1:A:1210:ILE:HD11	1:A:1214:ALA:HB2	2.01	0.41
1:A:1222:GLN:O	1:A:1224:PHE:N	2.54	0.41
1:A:745:ALA:O	1:A:746:PHE:C	2.64	0.41
1:A:1224:PHE:CA	1:A:1227:ARG:HB2	2.51	0.41
1:A:648:LEU:CG	1:A:763:PHE:CE1	3.03	0.40
1:A:656:LEU:HD22	1:A:751:LEU:O	2.19	0.40
1:A:1092:LEU:C	1:A:1094:ILE:N	2.79	0.40
1:A:434:PRO:HA	1:A:439:ILE:HG12	2.03	0.40
1:A:842:PHE:O	1:A:1136:VAL:HG11	2.21	0.40
1:A:893:LEU:O	1:A:896:GLY:N	2.54	0.40
1:A:1112:VAL:HA	1:A:1115:VAL:CG2	2.49	0.40
1:A:1234:LEU:HD22	1:A:1234:LEU:C	2.47	0.40
1:A:885:ALA:N	1:A:1079:PHE:O	2.51	0.40
1:A:926:ALA:C	1:A:1040:THR:HG22	2.29	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1126/1278 (88%)	898 (80%)	134 (12%)	94 (8%)	0 9

All (94) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	250	LYS
1	A	256	PRO
1	A	350	PRO
1	A	372	ARG
1	A	374	THR
1	A	376	ASN
1	A	403	PHE
1	A	638	ALA
1	A	639	LEU
1	A	642	MET
1	A	700	ASP
1	A	706	VAL
1	A	737	LEU
1	A	739	SER
1	A	829	LEU
1	A	856	VAL
1	A	864	LEU
1	A	876	PHE
1	A	922	GLN
1	A	929	LEU
1	A	930	ASP
1	A	951	LYS
1	A	957	CYS
1	A	958	ARG
1	A	1007	PRO
1	A	1008	ASN
1	A	1009	PRO
1	A	1010	LYS
1	A	1044	VAL
1	A	1071	ILE
1	A	1072	ASN
1	A	1083	VAL
1	A	1085	TYR
1	A	1086	VAL
1	A	1122	TRP
1	A	1146	GLY
1	A	260	TRP
1	A	475	TYR
1	A	605	ALA
1	A	606	GLU
1	A	617	SER
1	A	641	HIS

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Mol	Chain	Res	Type
1	A	760	PHE
1	A	830	LEU
1	A	888	PRO
1	A	923	ILE
1	A	943	ILE
1	A	1022	ALA
1	A	1073	GLY
1	A	1075	ALA
1	A	1177	VAL
1	A	1179	MET
1	A	1215	PHE
1	A	168	SER
1	A	348	ARG
1	A	498	LYS
1	A	668	VAL
1	A	861	ASP
1	A	877	LYS
1	A	890	TYR
1	A	894	GLU
1	A	1178	SER
1	A	1221	PHE
1	A	252	GLN
1	A	691	PRO
1	A	745	ALA
1	A	891	PHE
1	A	917	ASP
1	A	926	ALA
1	A	1084	PHE
1	A	1093	THR
1	A	1120	GLU
1	A	1150	ASN
1	A	1167	PHE
1	A	258	ALA
1	A	353	VAL
1	A	371	VAL
1	A	384	PRO
1	A	703	PHE
1	A	733	PRO
1	A	734	SER
1	A	925	ASN
1	A	1117	LEU
1	A	253	PRO

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Mol	Chain	Res	Type
1	A	259	PRO
1	A	401	PRO
1	A	880	SER
1	A	887	PRO
1	A	1080	PRO
1	A	166	PRO
1	A	892	VAL
1	A	1202	ILE
1	A	349	ASN
1	A	257	PRO

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	643/1109 (58%)	567 (88%)	76 (12%)	5 19

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	GLN
1	A	87	LEU
1	A	91	LEU
1	A	105	LEU
1	A	116	ARG
1	A	164	GLU
1	A	196	LYS
1	A	250	LYS
1	A	252	GLN
1	A	381	TRP
1	A	389	ARG
1	A	394	TYR
1	A	398	HIS
1	A	399	PHE
1	A	404	ARG
1	A	406	GLU

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Mol	Chain	Res	Type
1	A	439	ILE
1	A	472	LEU
1	A	495	LEU
1	A	518	ARG
1	A	526	THR
1	A	592	LYS
1	A	602	SER
1	A	607	ARG
1	A	612	GLU
1	A	648	LEU
1	A	653	LYS
1	A	662	LEU
1	A	676	SER
1	A	680	LEU
1	A	682	LEU
1	A	684	LEU
1	A	685	ILE
1	A	688	GLU
1	A	718	GLU
1	A	719	THR
1	A	722	GLN
1	A	730	GLU
1	A	751	LEU
1	A	758	HIS
1	A	760	PHE
1	A	1036	THR
1	A	1037	TYR
1	A	1038	PHE
1	A	1039	MET
1	A	1041	TYR
1	A	1050	ASP
1	A	1055	LEU
1	A	1056	LYS
1	A	1057	LYS
1	A	1059	ARG
1	A	1066	THR
1	A	1069	MET
1	A	1072	ASN
1	A	1074	SER
1	A	1082	SER
1	A	1084	PHE
1	A	1090	GLN

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Mol	Chain	Res	Type
1	A	1117	LEU
1	A	1127	MET
1	A	1128	CYS
1	A	1138	MET
1	A	1153	SER
1	A	1154	LEU
1	A	1159	MET
1	A	1166	GLU
1	A	1172	THR
1	A	1173	ARG
1	A	1186	ARG
1	A	1189	GLU
1	A	1194	MET
1	A	1199	PHE
1	A	1207	PHE
1	A	1227	ARG
1	A	1228	MET
1	A	1234	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	70	ASN
1	A	92	GLN
1	A	135	ASN
1	A	154	ASN
1	A	185	ASN
1	A	200	GLN
1	A	241	GLN
1	A	452	ASN
1	A	459	ASN
1	A	465	GLN
1	A	478	ASN
1	A	510	HIS
1	A	598	ASN
1	A	722	GLN
1	A	1072	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

13 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	NAG	B	1	2,1	14,14,15	0.68	0	17,19,21	1.11	1 (5%)
2	NAG	B	2	2	14,14,15	0.56	0	17,19,21	0.74	1 (5%)
2	NAG	C	1	2	14,14,15	0.48	0	17,19,21	1.47	3 (17%)
2	NAG	C	2	2	14,14,15	0.29	0	17,19,21	0.57	0
3	NAG	D	1	3	14,14,15	0.30	0	17,19,21	0.48	0
3	NAG	D	2	3	14,14,15	0.30	0	17,19,21	0.55	0
3	BMA	D	3	3	11,11,12	0.26	0	15,15,17	0.52	0
2	NAG	E	1	2	14,14,15	0.35	0	17,19,21	1.56	3 (17%)
2	NAG	E	2	2	14,14,15	0.68	1 (7%)	17,19,21	1.06	1 (5%)
4	NAG	F	1	4	14,14,15	0.28	0	17,19,21	0.56	0
4	NAG	F	2	4	14,14,15	0.28	0	17,19,21	0.78	0
4	BMA	F	3	4	11,11,12	0.28	0	15,15,17	0.64	0
4	MAN	F	4	4	11,11,12	0.36	0	15,15,17	1.02	1 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	1	2,1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	2	2	-	0/6/23/26	0/1/1/1
2	NAG	C	1	2	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	3/6/23/26	0/1/1/1
3	NAG	D	1	3	-	5/6/23/26	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1
3	BMA	D	3	3	-	2/2/19/22	0/1/1/1
2	NAG	E	1	2	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	1/6/23/26	0/1/1/1
4	NAG	F	1	4	-	2/6/23/26	0/1/1/1
4	NAG	F	2	4	-	0/6/23/26	0/1/1/1
4	BMA	F	3	4	-	0/2/19/22	0/1/1/1
4	MAN	F	4	4	-	2/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	2	NAG	C1-C2	2.09	1.55	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	NAG	O5-C1-C2	-4.37	104.53	111.29
2	E	1	NAG	C1-O5-C5	3.46	116.82	112.19
2	E	1	NAG	O4-C4-C3	-3.24	102.75	110.38
4	F	4	MAN	C1-C2-C3	2.93	113.91	109.64
2	E	2	NAG	C4-C3-C2	2.85	115.19	111.02
2	C	1	NAG	C4-C3-C2	2.68	114.94	111.02
2	B	1	NAG	O5-C1-C2	-2.58	107.30	111.29
2	E	1	NAG	O5-C1-C2	-2.51	107.40	111.29
2	C	1	NAG	C1-O5-C5	2.24	115.18	112.19
2	B	2	NAG	C1-O5-C5	2.20	115.14	112.19

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	1	NAG	C1-C2-N2-C7
3	D	1	NAG	C8-C7-N2-C2
3	D	1	NAG	O7-C7-N2-C2
3	D	2	NAG	C8-C7-N2-C2

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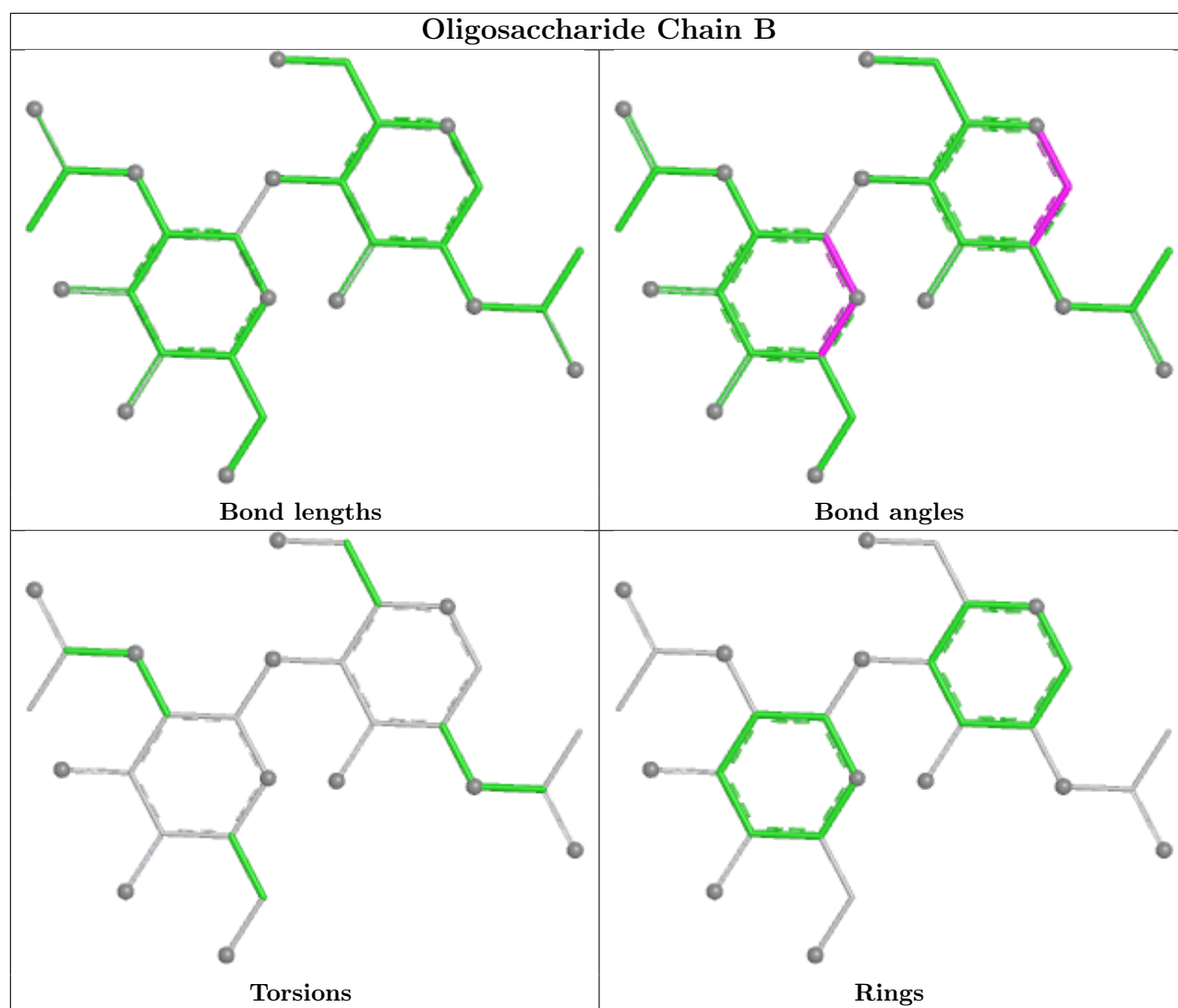
Mol	Chain	Res	Type	Atoms
3	D	2	NAG	O7-C7-N2-C2
2	C	2	NAG	O5-C5-C6-O6
4	F	4	MAN	O5-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
4	F	4	MAN	C4-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6
3	D	3	BMA	O5-C5-C6-O6
4	F	1	NAG	O5-C5-C6-O6
3	D	3	BMA	C4-C5-C6-O6
3	D	1	NAG	C4-C5-C6-O6
3	D	1	NAG	O5-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6
4	F	1	NAG	C4-C5-C6-O6
2	C	2	NAG	C3-C2-N2-C7
2	E	2	NAG	C3-C2-N2-C7

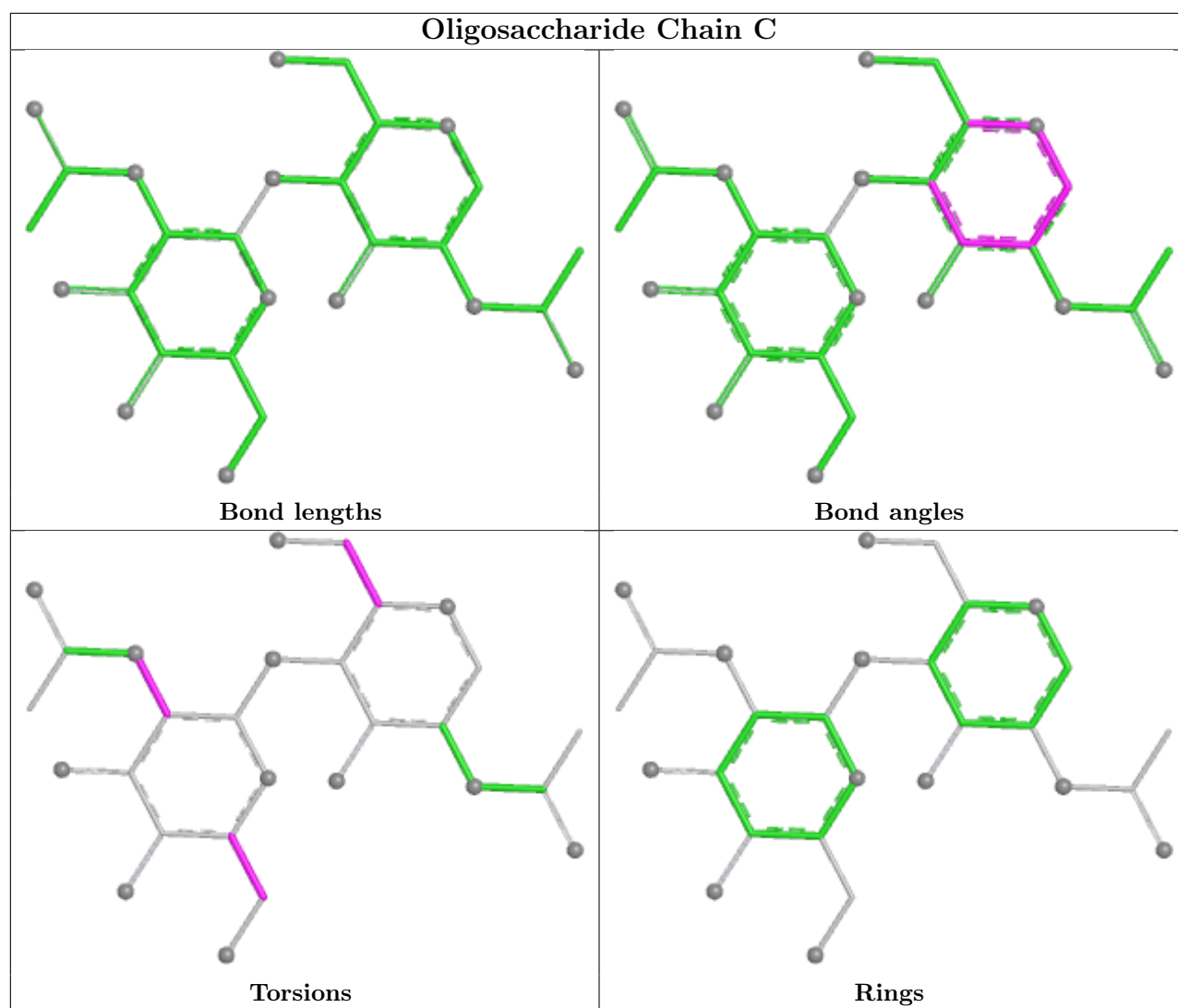
There are no ring outliers.

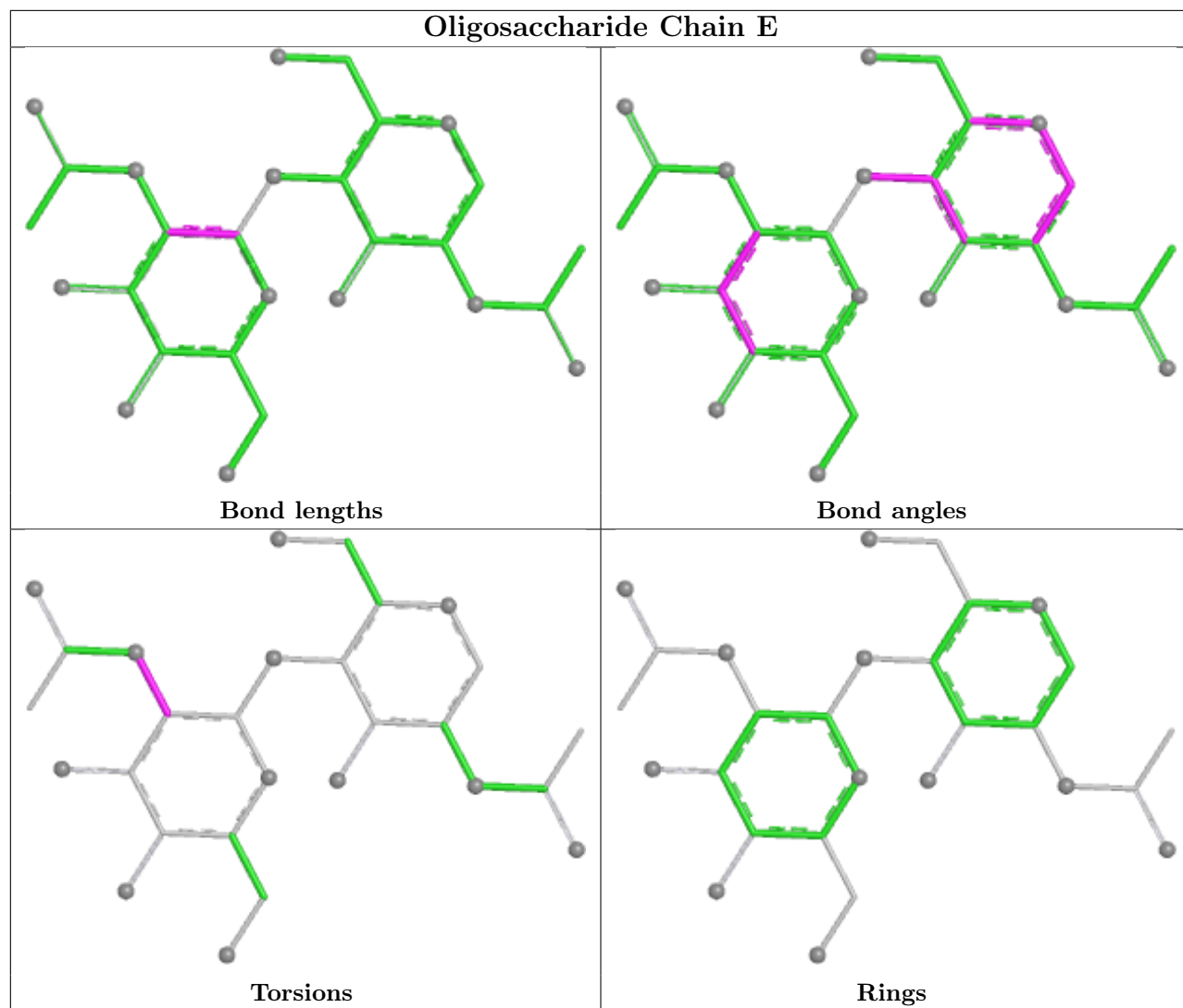
9 monomers are involved in 36 short contacts:

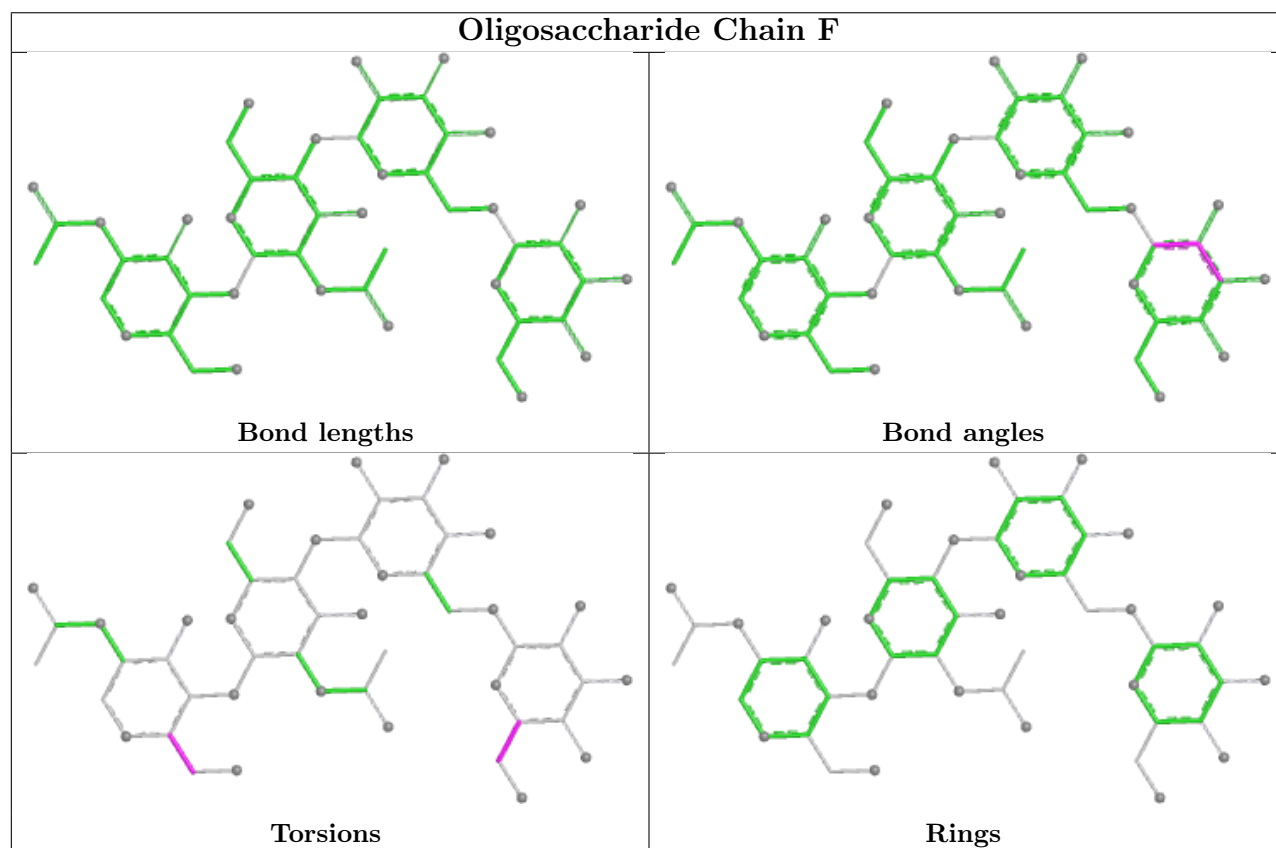
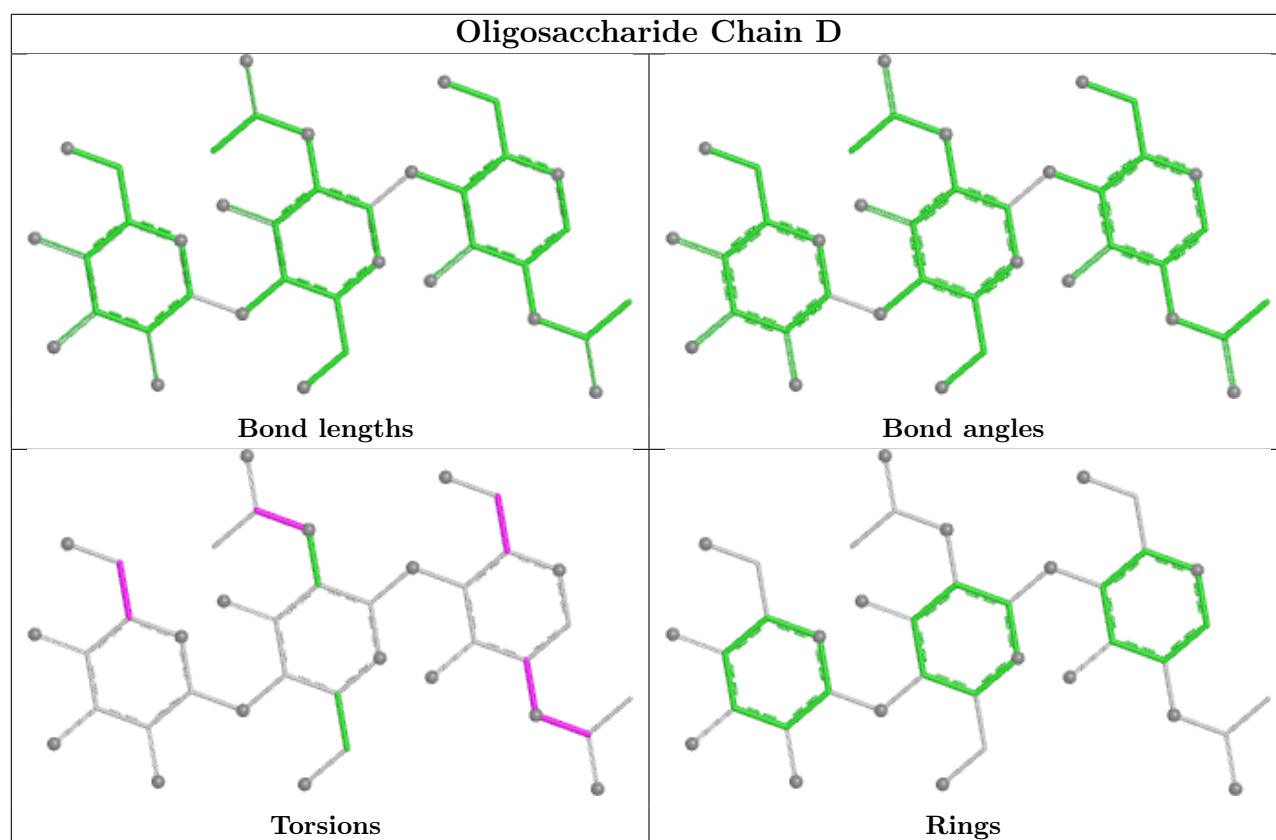
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1	NAG	15	0
4	F	2	NAG	6	0
2	E	1	NAG	4	0
4	F	1	NAG	8	0
2	C	2	NAG	1	0
3	D	2	NAG	13	0
3	D	3	BMA	4	0
4	F	3	BMA	2	0
2	C	1	NAG	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.









5.6 Ligand geometry

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	NAG	A	1303	-	14,14,15	0.31	0	17,19,21	0.56	0
5	NAG	A	1318	-	14,14,15	0.42	0	17,19,21	1.15	2 (11%)
5	NAG	A	1322	-	14,14,15	0.30	0	17,19,21	0.56	0
5	NAG	A	1316	1	14,14,15	0.44	0	17,19,21	1.16	2 (11%)
5	NAG	A	1321	-	14,14,15	0.30	0	17,19,21	0.57	0
5	NAG	A	1323	-	14,14,15	0.29	0	17,19,21	0.56	0
5	NAG	A	1309	-	14,14,15	0.51	0	17,19,21	1.14	2 (11%)
6	CLR	A	1325	-	31,31,31	0.60	0	48,48,48	1.59	8 (16%)
5	NAG	A	1320	1	14,14,15	0.30	0	17,19,21	0.56	0
5	NAG	A	1324	-	14,14,15	0.44	0	17,19,21	1.17	2 (11%)
5	NAG	A	1319	-	14,14,15	0.41	0	17,19,21	1.16	2 (11%)
5	NAG	A	1317	-	14,14,15	0.29	0	17,19,21	0.56	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	1303	-	-	5/6/23/26	0/1/1/1
5	NAG	A	1318	-	-	0/6/23/26	0/1/1/1
5	NAG	A	1322	-	-	2/6/23/26	0/1/1/1
5	NAG	A	1316	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1321	-	-	0/6/23/26	0/1/1/1
5	NAG	A	1323	-	-	4/6/23/26	0/1/1/1
5	NAG	A	1309	-	-	0/6/23/26	0/1/1/1
6	CLR	A	1325	-	-	0/10/68/68	0/4/4/4
5	NAG	A	1320	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1324	-	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	1319	-	-	0/6/23/26	0/1/1/1
5	NAG	A	1317	-	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1325	CLR	C1-C10-C9	3.72	113.65	108.74
6	A	1325	CLR	C1-C2-C3	-3.53	105.81	110.48
6	A	1325	CLR	C14-C8-C9	3.42	113.55	109.09
6	A	1325	CLR	C8-C7-C6	-3.15	108.39	112.76
6	A	1325	CLR	C4-C5-C6	-3.05	116.44	120.57
6	A	1325	CLR	C3-C4-C5	-2.92	107.40	112.05
6	A	1325	CLR	C4-C5-C10	2.50	119.62	116.42
5	A	1319	NAG	C8-C7-N2	2.34	120.00	116.12
5	A	1318	NAG	C8-C7-N2	2.32	119.97	116.12
5	A	1324	NAG	C8-C7-N2	2.32	119.97	116.12
5	A	1316	NAG	C8-C7-N2	2.31	119.94	116.12
6	A	1325	CLR	C18-C13-C17	-2.27	107.55	111.68
5	A	1324	NAG	C2-N2-C7	-2.21	119.93	122.90
5	A	1318	NAG	C2-N2-C7	-2.20	119.95	122.90
5	A	1316	NAG	C2-N2-C7	-2.19	119.97	122.90
5	A	1319	NAG	C2-N2-C7	-2.18	119.97	122.90
5	A	1309	NAG	C1-C2-N2	-2.10	107.12	110.43
5	A	1309	NAG	C8-C7-N2	-2.03	112.76	116.12

There are no chirality outliers.

All (11) torsion outliers are listed below:

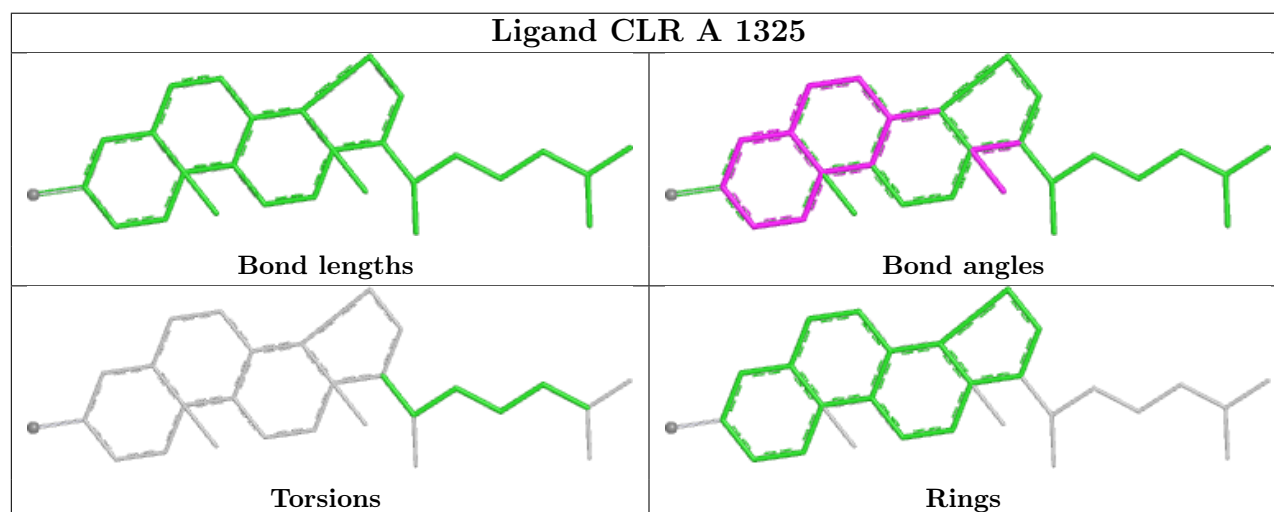
Mol	Chain	Res	Type	Atoms
5	A	1303	NAG	C8-C7-N2-C2
5	A	1303	NAG	O7-C7-N2-C2
5	A	1322	NAG	C8-C7-N2-C2
5	A	1322	NAG	O7-C7-N2-C2
5	A	1323	NAG	C8-C7-N2-C2
5	A	1323	NAG	O7-C7-N2-C2
5	A	1323	NAG	O5-C5-C6-O6
5	A	1303	NAG	O5-C5-C6-O6
5	A	1323	NAG	C4-C5-C6-O6
5	A	1303	NAG	C4-C5-C6-O6
5	A	1303	NAG	C3-C2-N2-C7

There are no ring outliers.

7 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1303	NAG	2	0
5	A	1322	NAG	4	0
5	A	1323	NAG	2	0
6	A	1325	CLR	1	0
5	A	1324	NAG	3	0
5	A	1319	NAG	4	0
5	A	1317	NAG	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	940:SER	C	941:SER	N	1.66

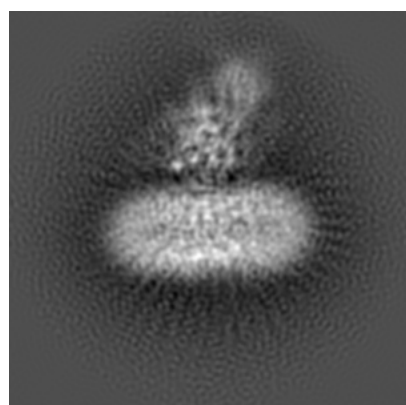
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6640. These allow visual inspection of the internal detail of the map and identification of artifacts.

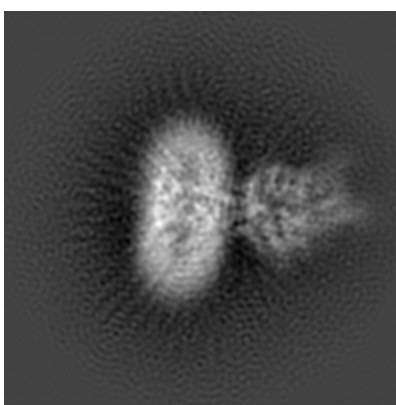
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

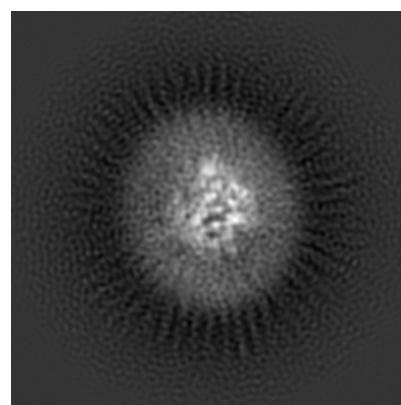
6.1.1 Primary map



X



Y

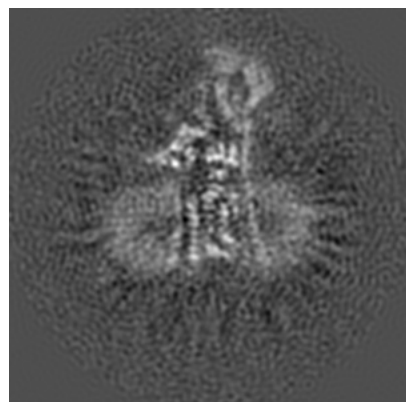


Z

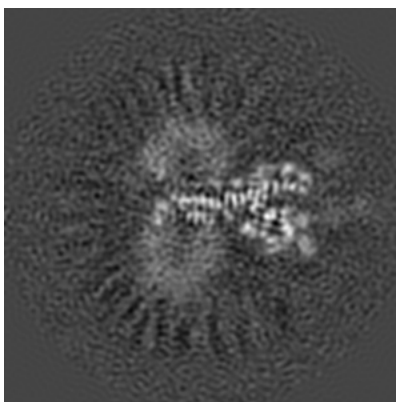
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

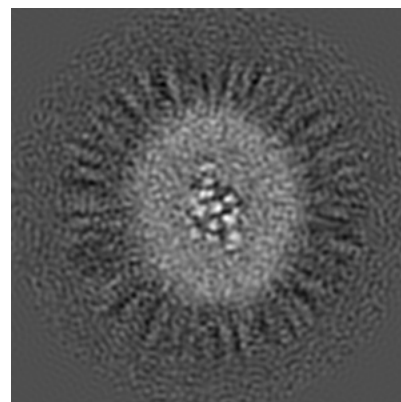
6.2.1 Primary map



X Index: 100



Y Index: 100

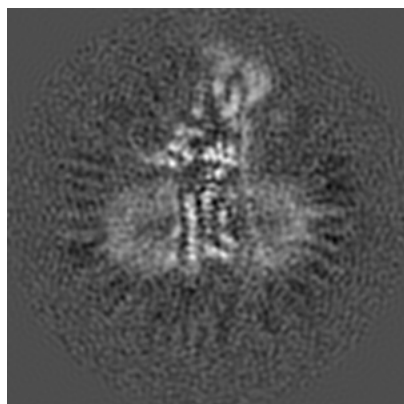


Z Index: 100

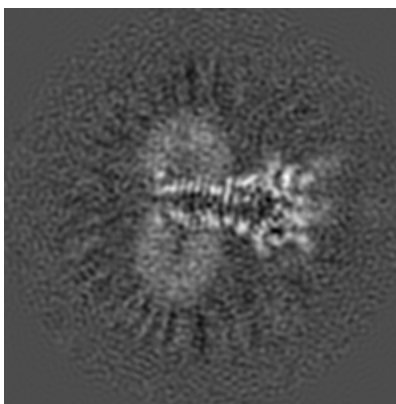
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

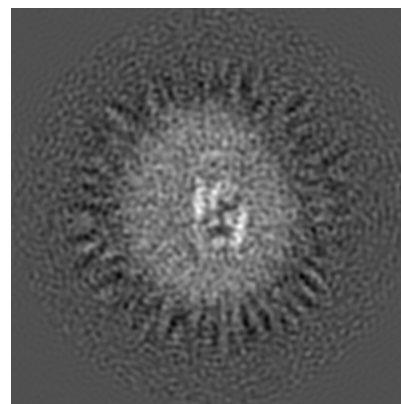
6.3.1 Primary map



X Index: 101



Y Index: 96

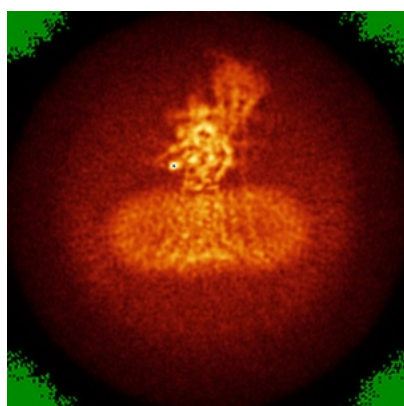


Z Index: 77

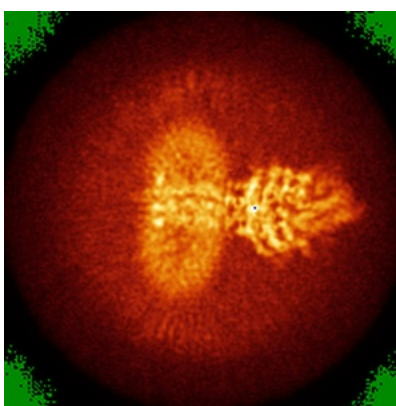
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

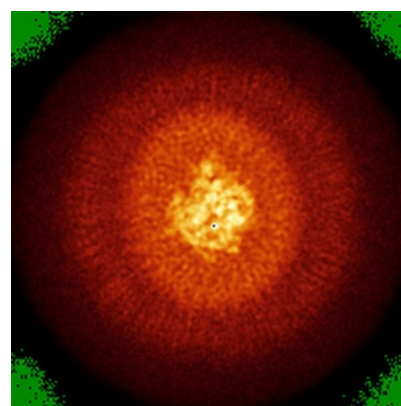
6.4.1 Primary map



X



Y

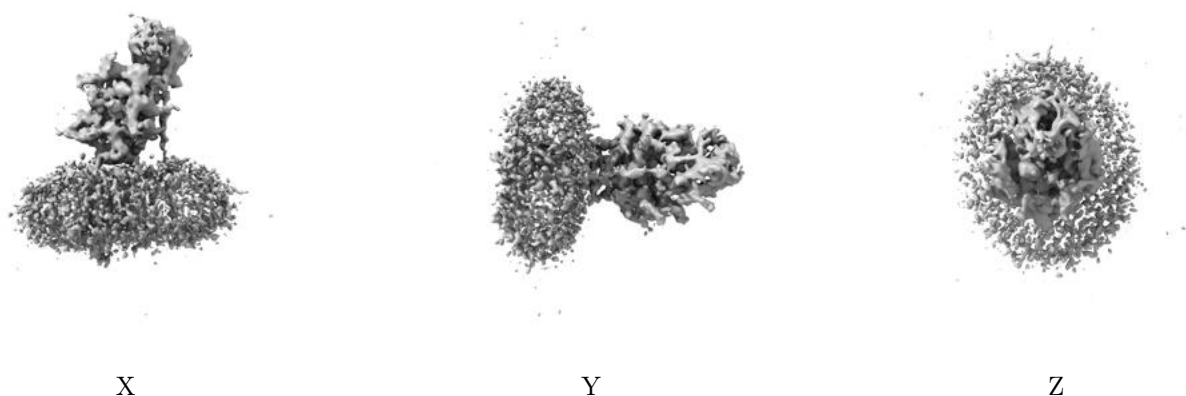


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

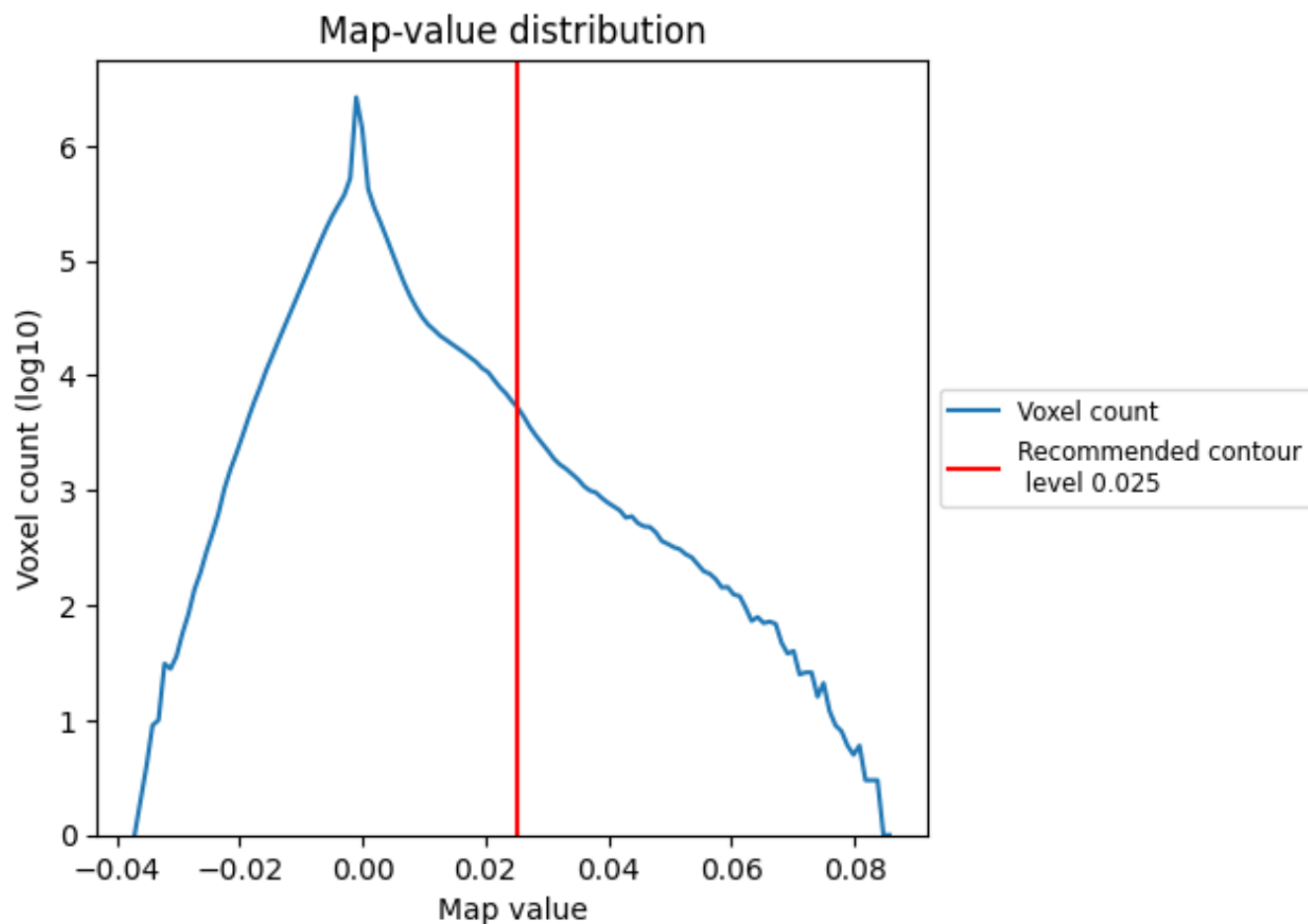
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

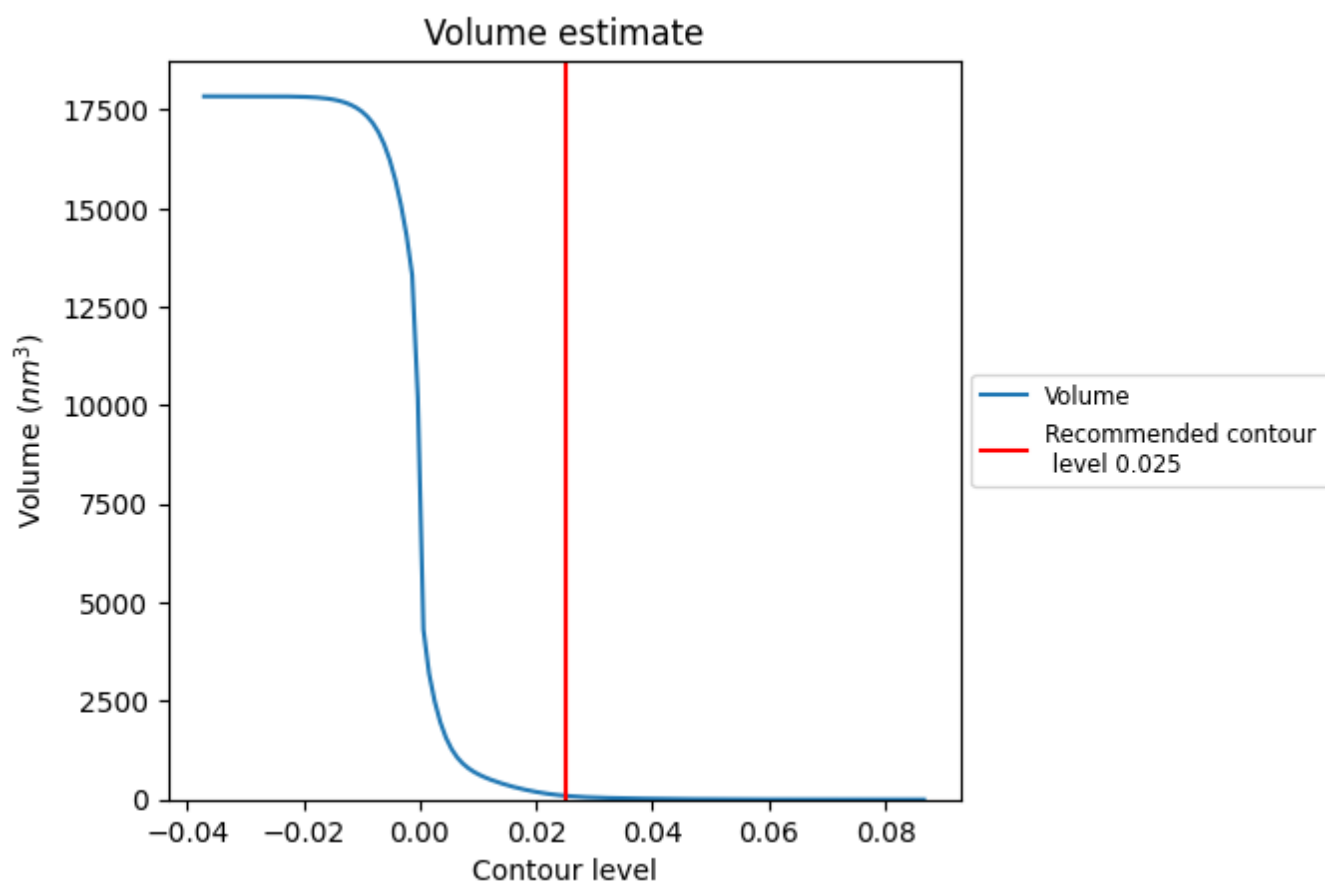
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

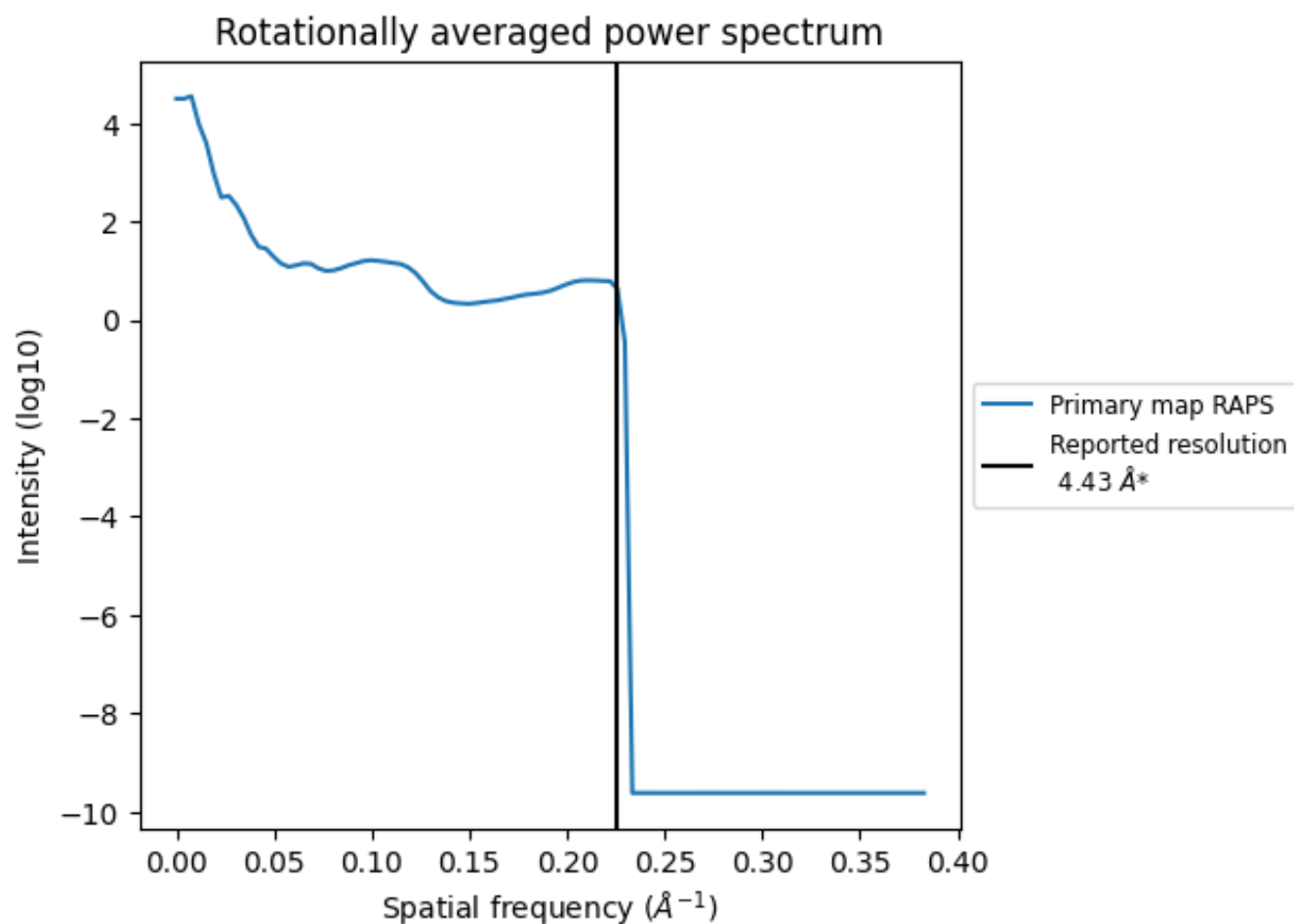
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 97 nm³; this corresponds to an approximate mass of 87 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.226 Å⁻¹

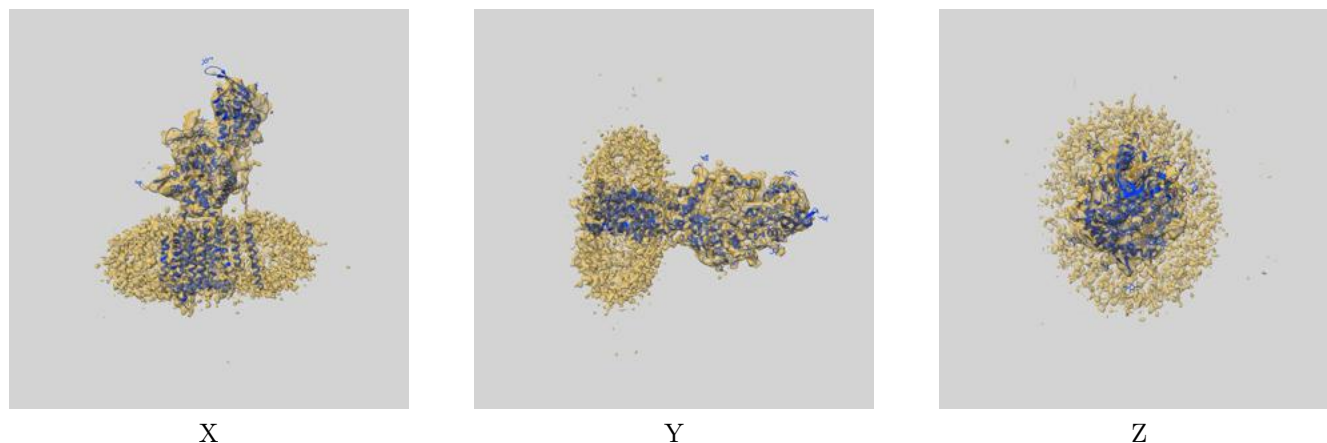
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

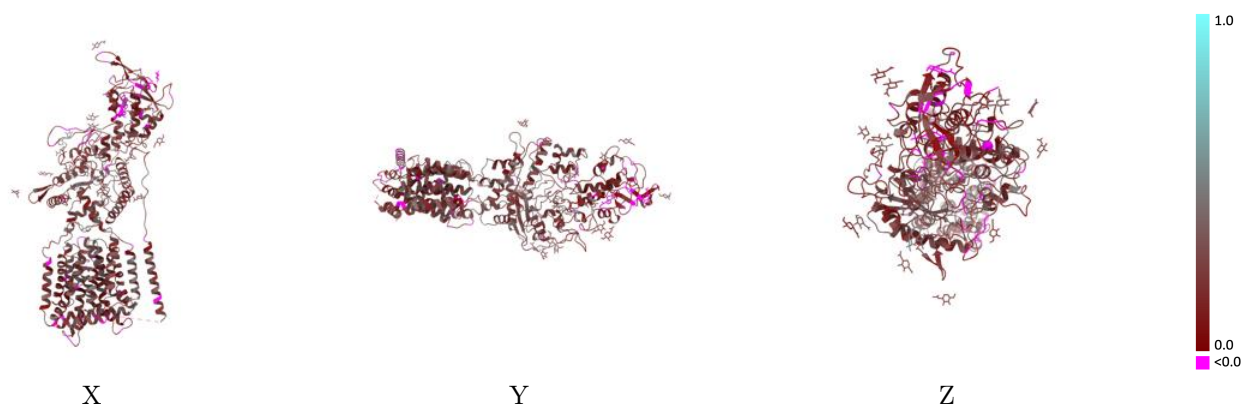
This section contains information regarding the fit between EMDB map EMD-6640 and PDB model 3JD8. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



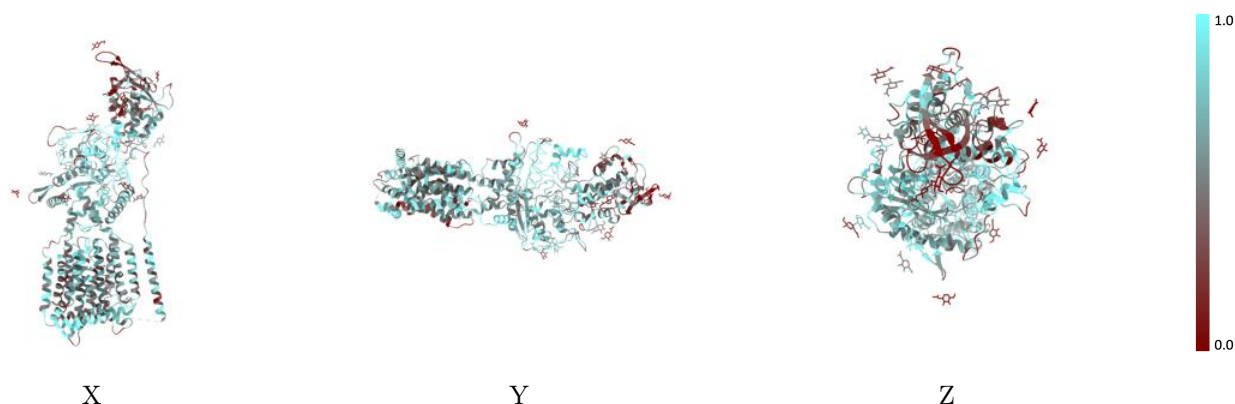
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



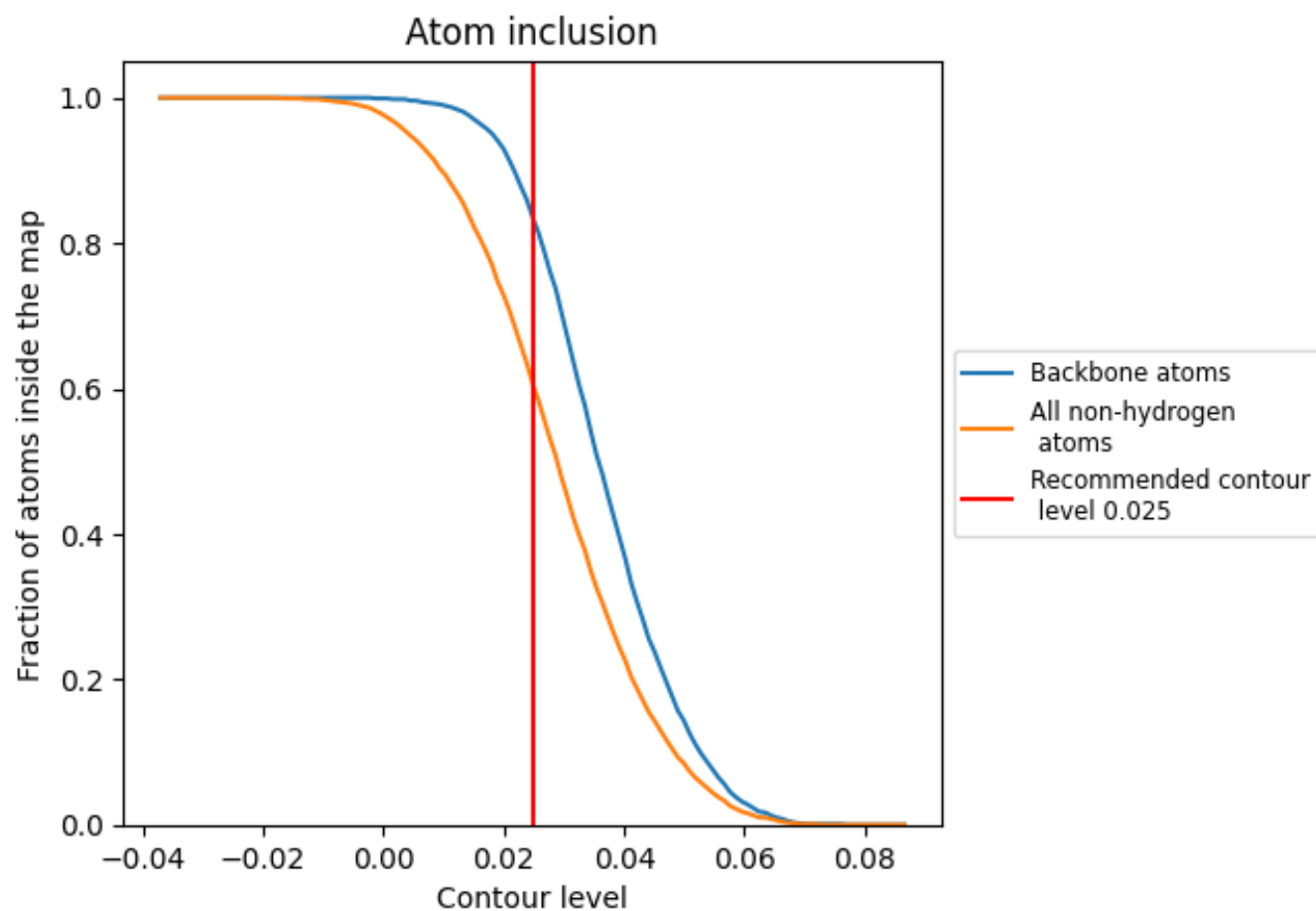
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.025).

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 60% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6020	0.2240
A	0.6030	0.2220
B	0.3570	0.2420
C	0.3210	0.3030
D	0.6410	0.2870
E	0.5000	0.2060
F	0.7400	0.4140

1.0

0.0

<0.0